2.830J / 6.780J / ESD.63J Control of Manufacturing Processes (SMA 6303)
Spring 2008

Modeling the embossing/imprinting of thermoplastic layers

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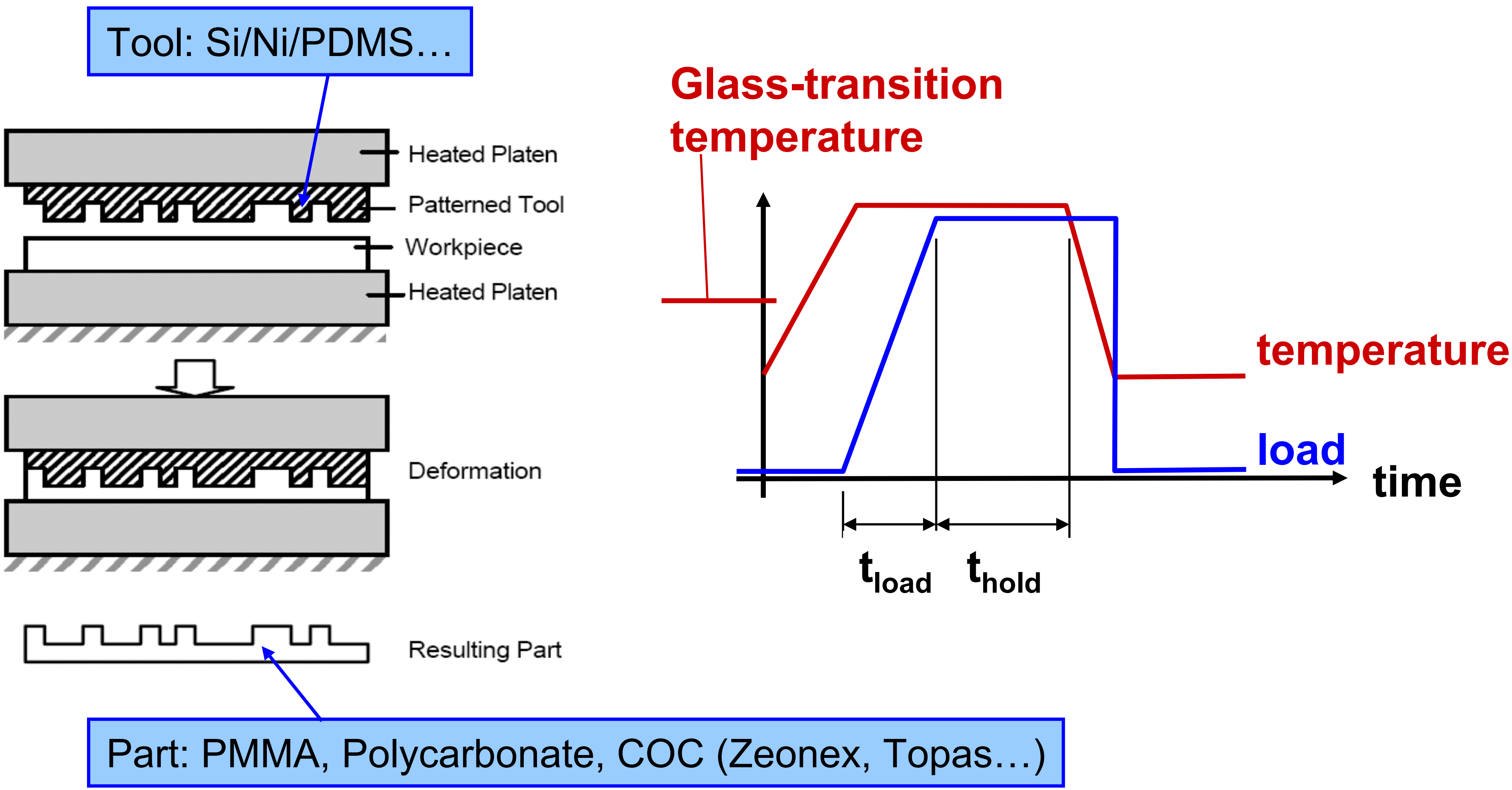
8 May 2008

Hot micro- and nano-embossing

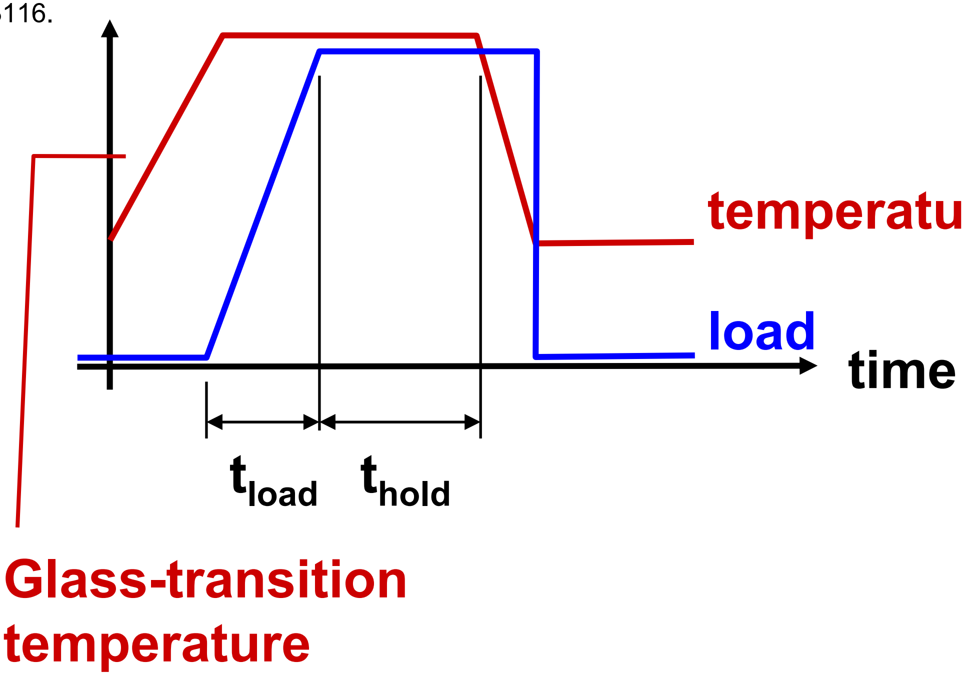


Applications: microfluidics, optics…

Thermal nanoimprint lithography (NIL): the process

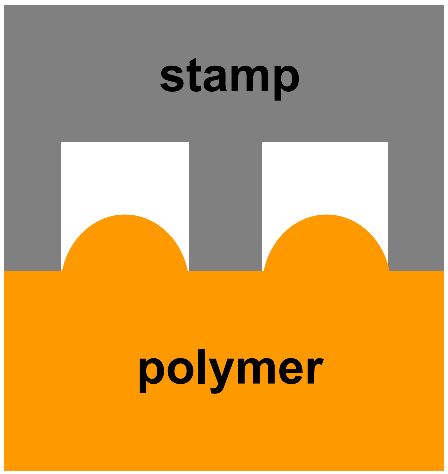
Applications: sub-100 nm lithography

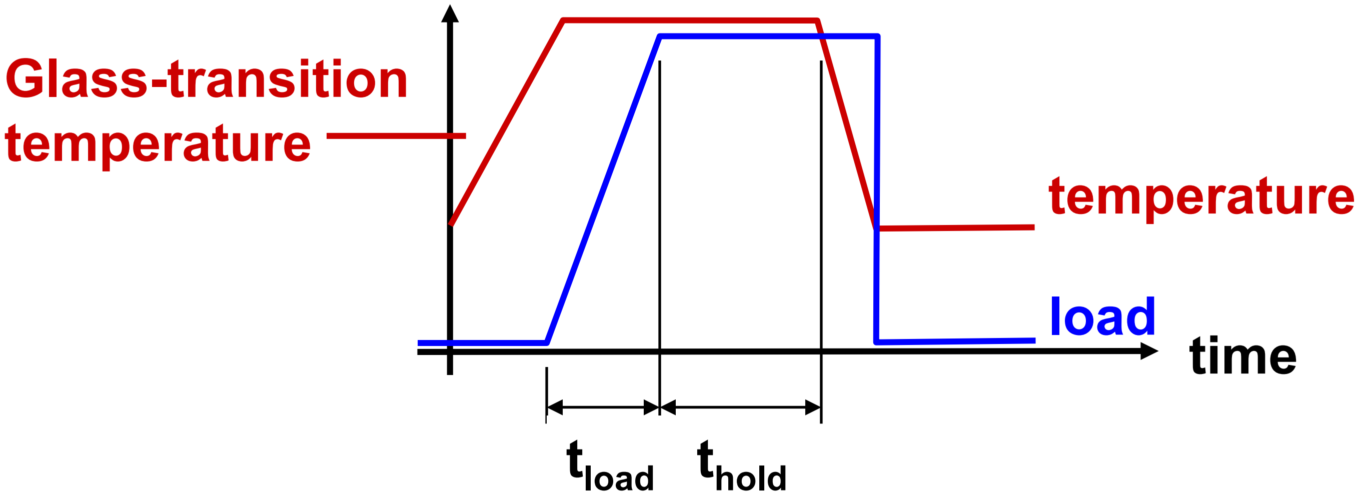
Image removed due to copyright restrictions. Please see Fig. 1 in Chou, Stephen Y., et al. “Imprint of sub-25 nm vias and Trenches in Polymers.” *Applied Physical Letters* 67 (November 1995): 3114-3116.



S.Y. Chou *et al., Appl. Phys. Lett.* vol. 67 pp. 3114-3116, 1995

Hot micro- and nano-embossing

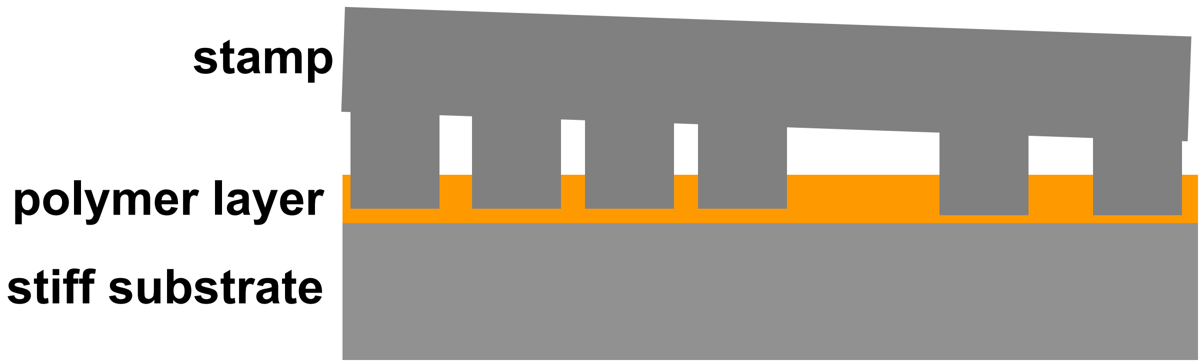




- **To choose an optimal process, we need to assign values to**
  - Temperature, load, times
- **Load and temperature are constrained by**
  - Equipment
  - Stamp and substrate properties
- **Our choice of substrate and pattern design are more or less constrained by the application**

Hot embossing: modeling aims

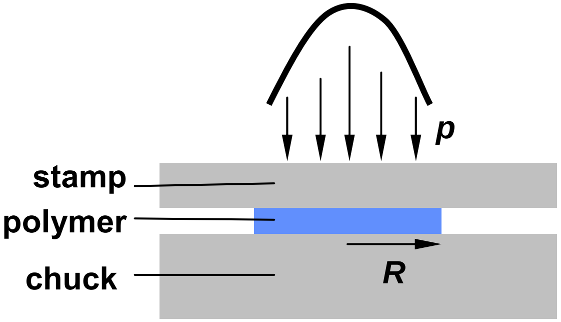
- How long to form a given set of features?
- How to improve pattern/process to reduce time or energy required?
- How to maximize uniformity of any residual layer?

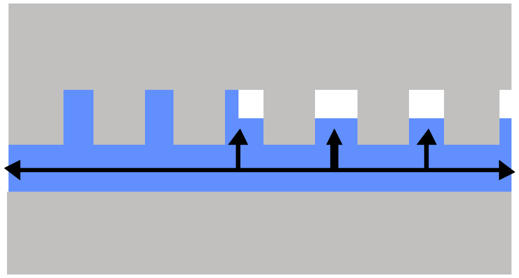


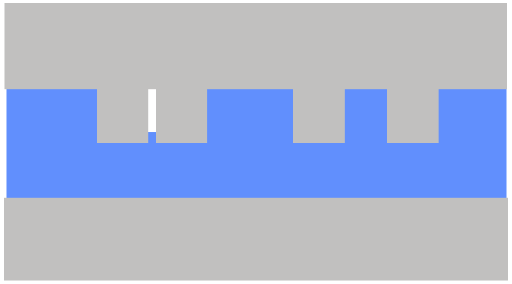
Non-uniformity occurs at three length scales

Spatial non-uniformity

- **Substrate- or machine-scale**
- **Device-scale; pattern-dependent**
- **Feature-scale**



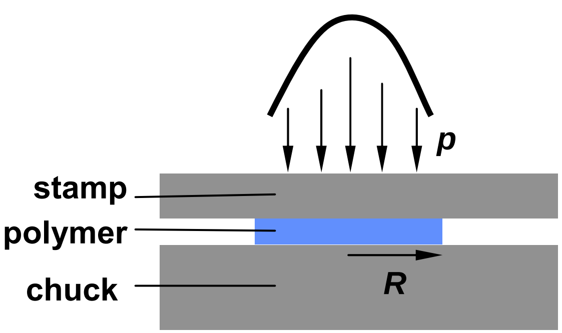


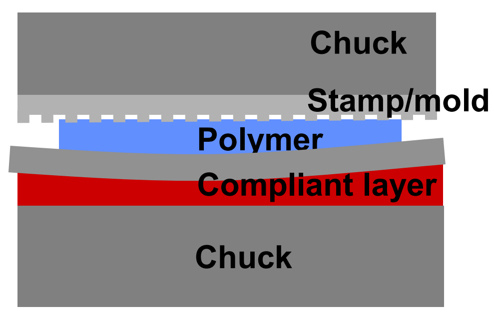


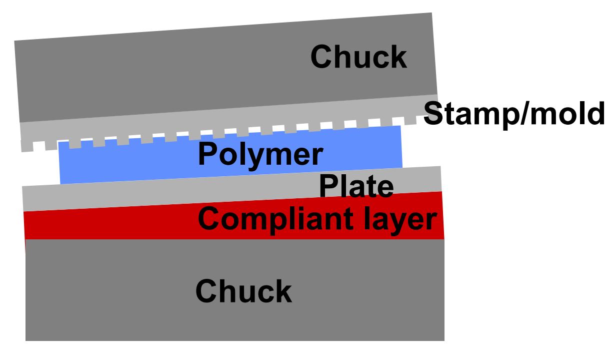
Workpiece-/machine-scale effects

Spatial non-uniformity

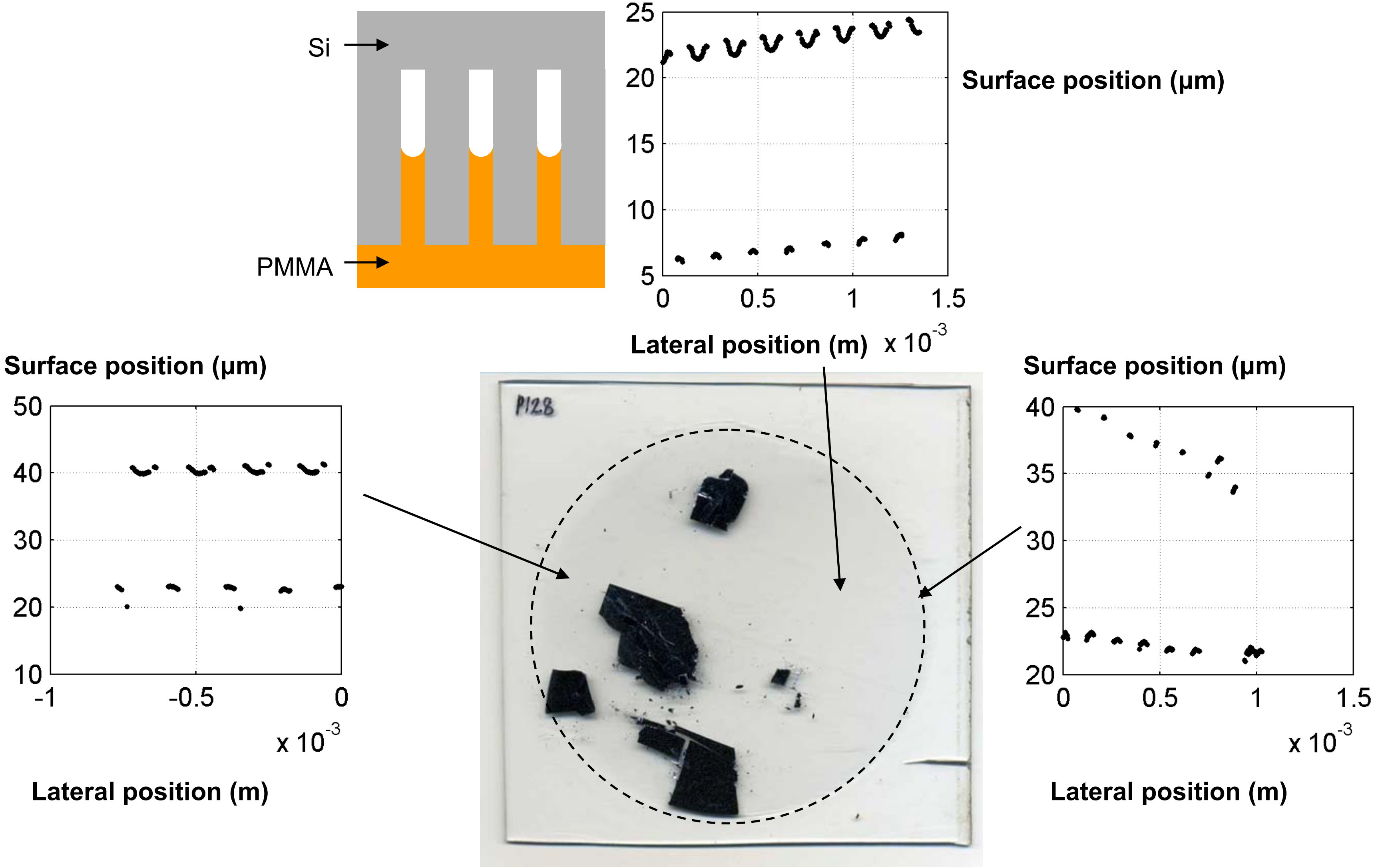
- **Substrate- or machine-scale**
  - **Pressure variation**
  - **Stamp/machine deflection**
  - **Imperfect parallelism**
- Device-scale; pattern-dependent
- Feature-scale



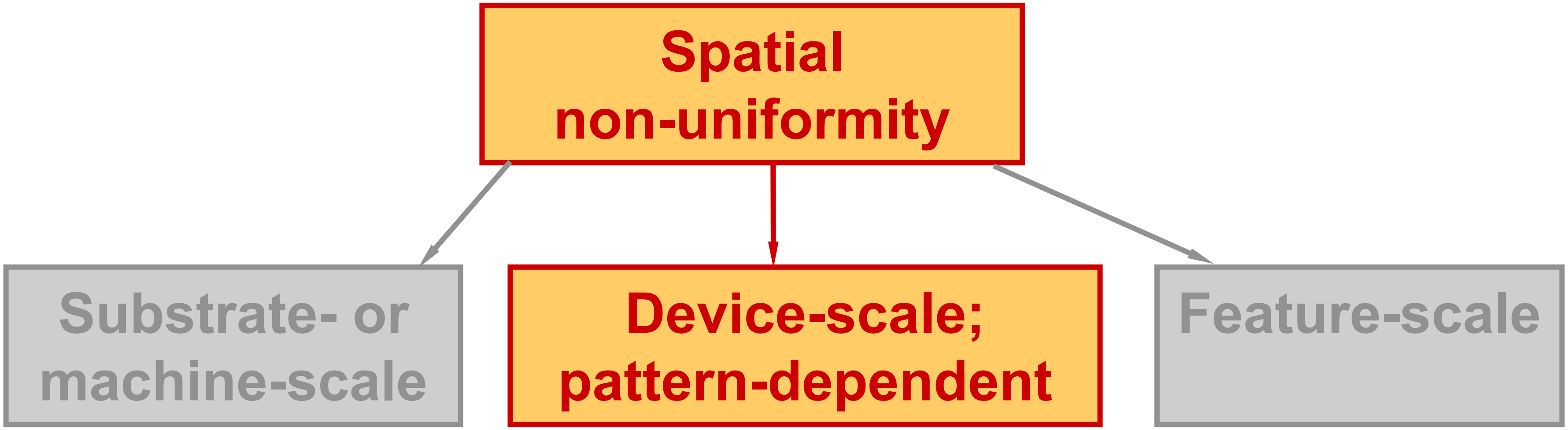




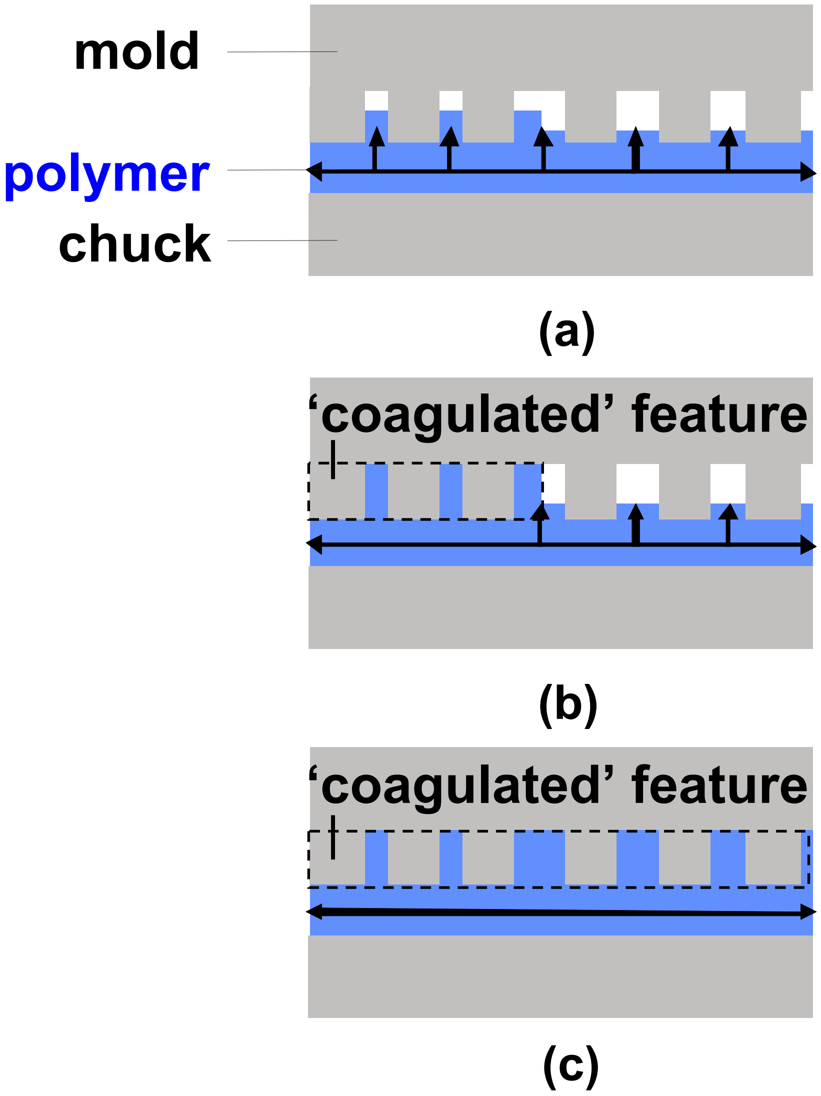
Workpiece-/machine-scale effects



Pattern-dependent non-uniformity



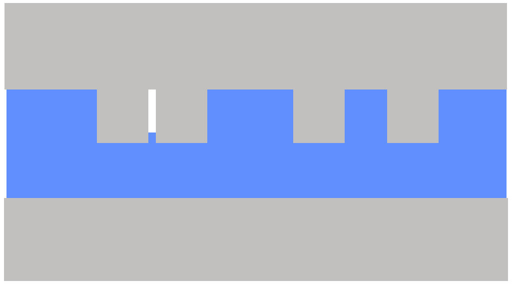
Pattern-dependent non-uniformity



Non-uniformity occurs at three length scales

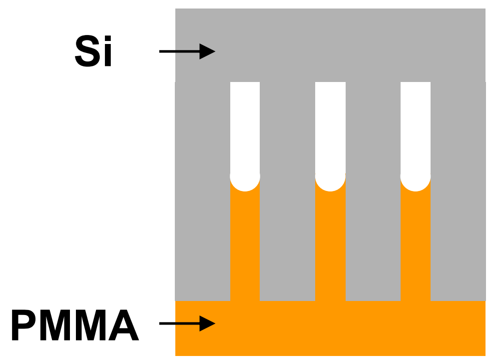
Spatial non-uniformity

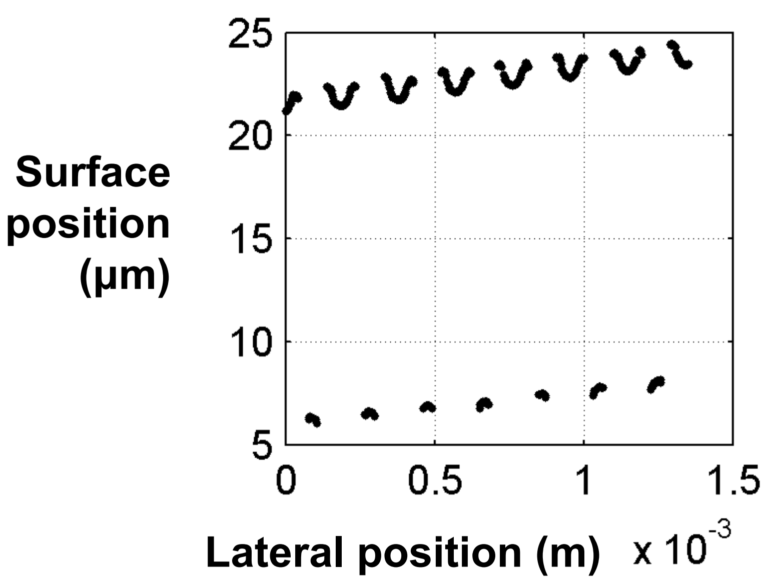
- Substrate- or machine-scale
- Device-scale; pattern-dependent
- **Feature-scale**



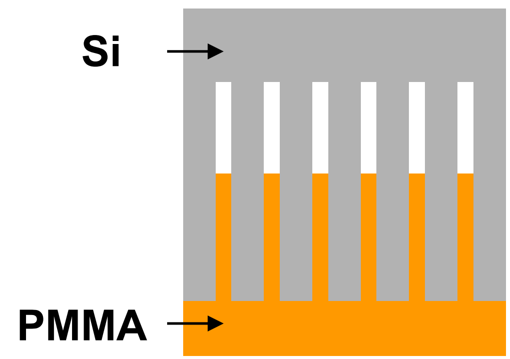
Feature-scale non-uniformity

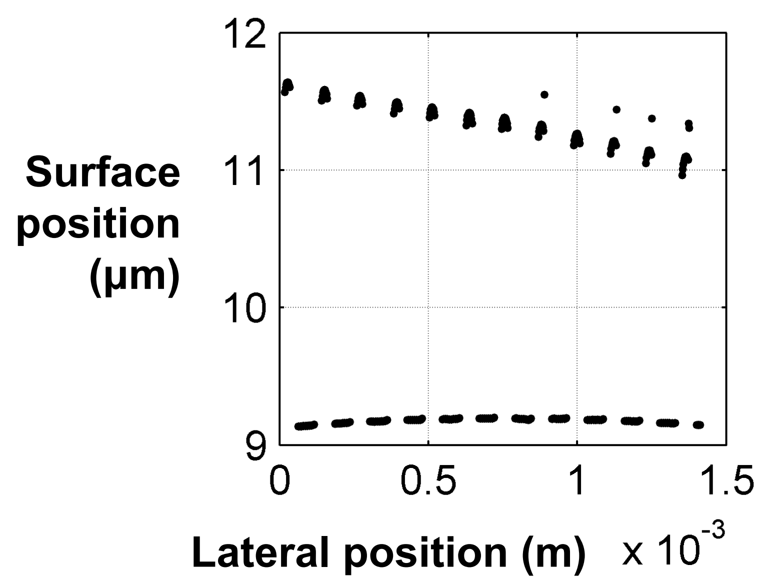
Larger-diameter features





Smaller-diameter features

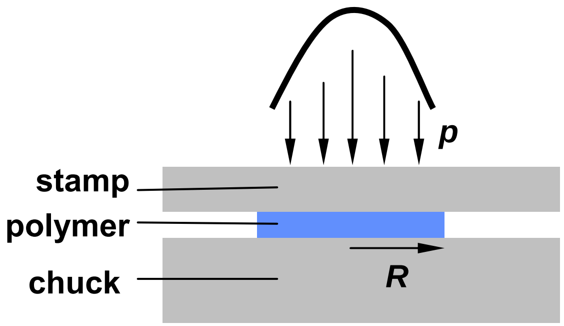


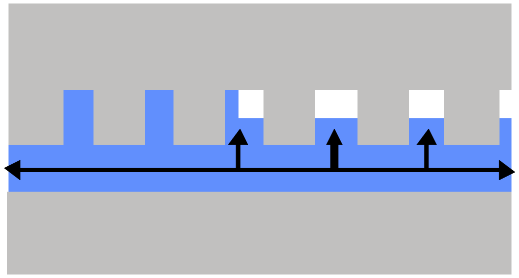


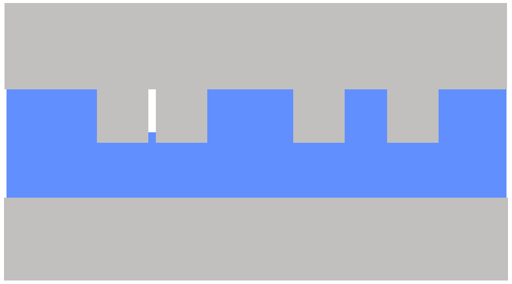
How to address effects at all three scales?

Spatial non-uniformity

- **Substrate- or machine-scale**
- **Device-scale; pattern-dependent**
- **Feature-scale**



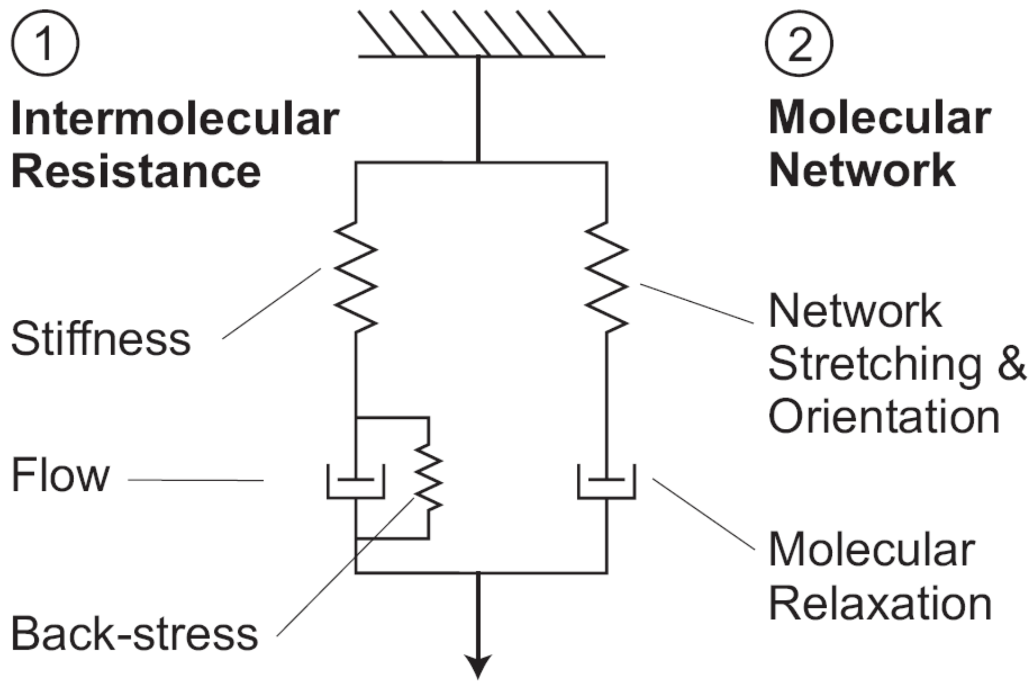




Parameters affecting the embossing outcome

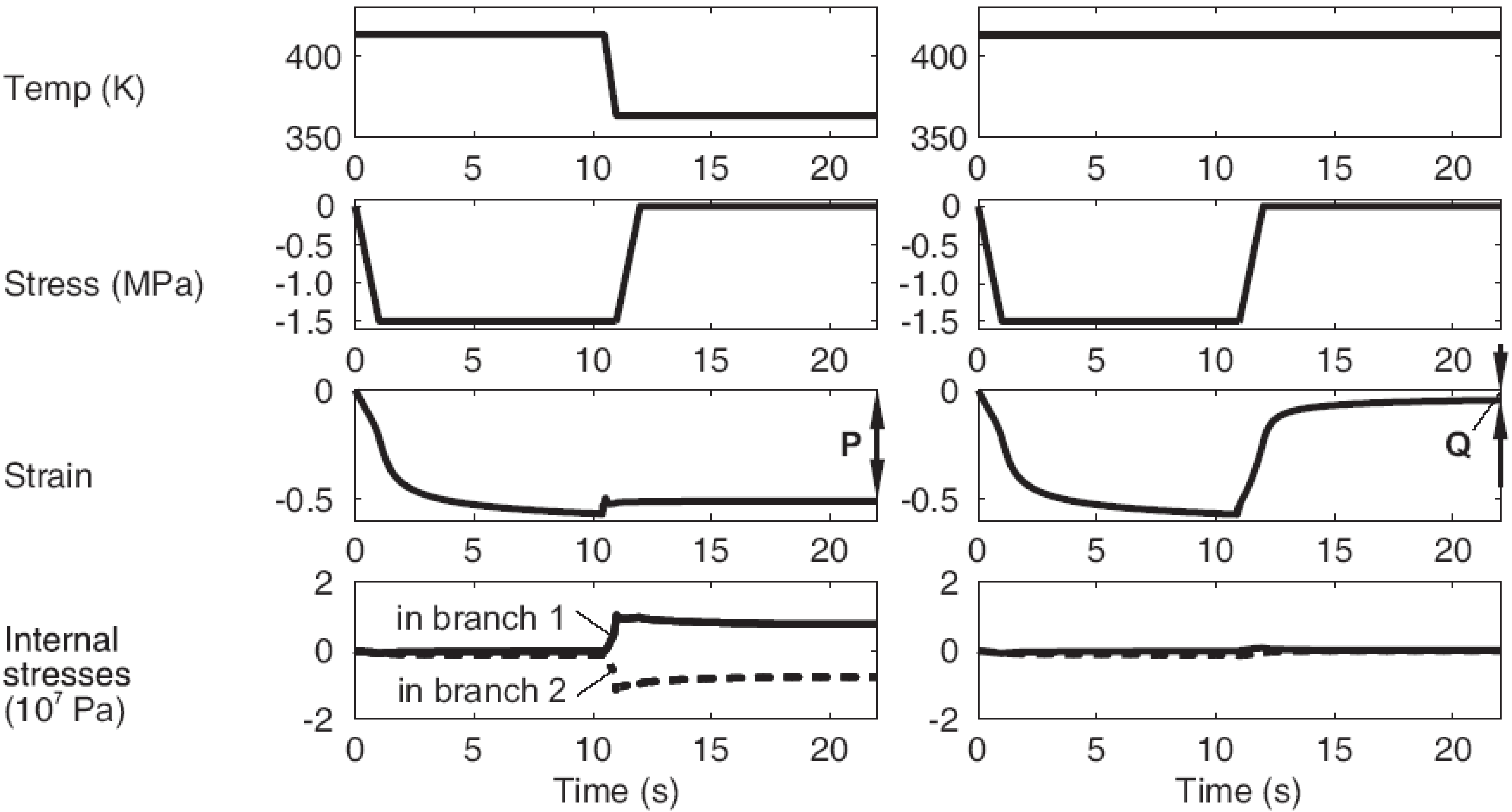
- Embossed pattern
  - Feature shapes, sizes, orientations
- Substrate
  - Material (type, molecular weight)
  - Thickness
- Process parameters
  - Temperature, pressure, hold time, …

PMMA in compression



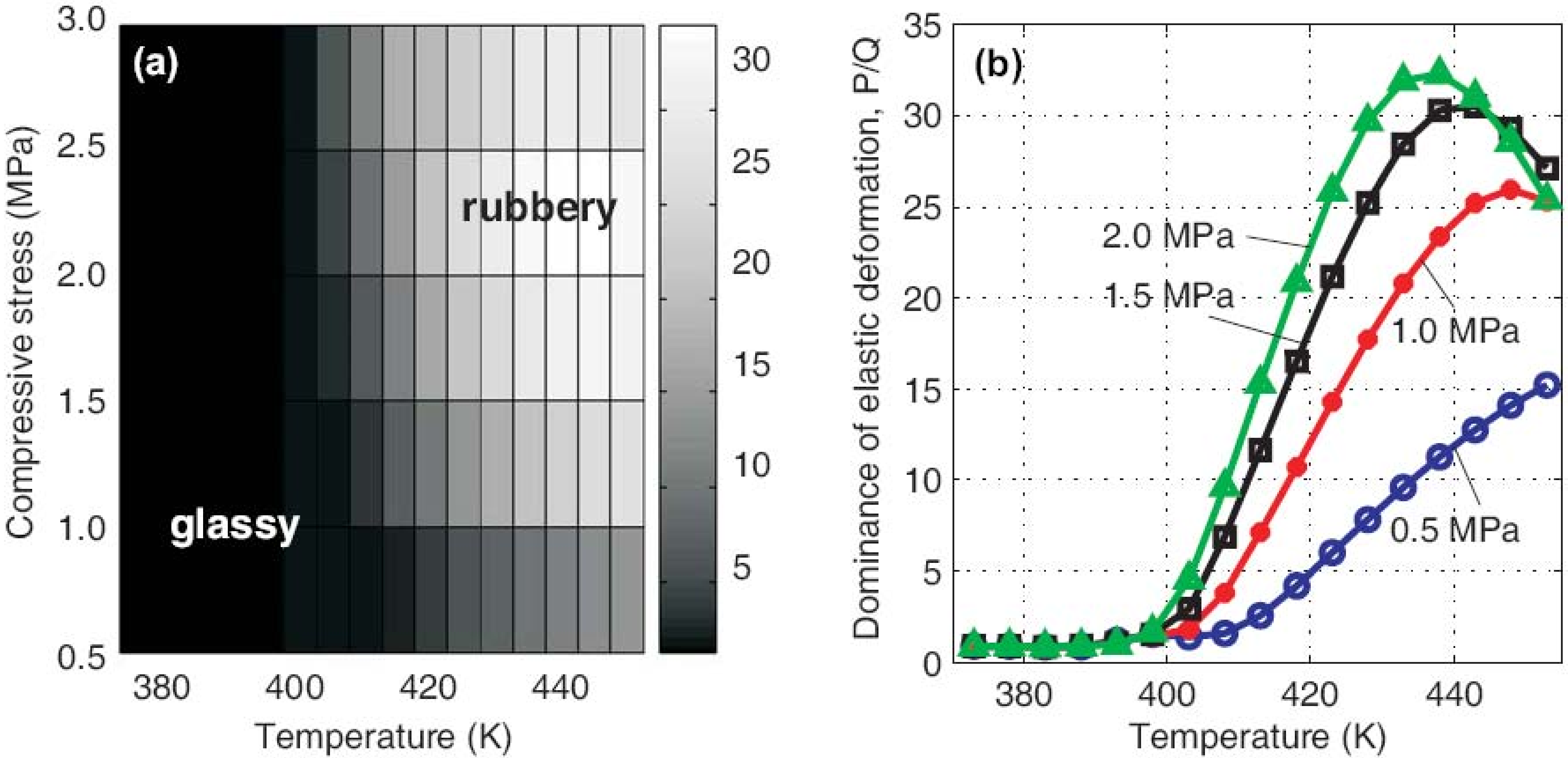
N.M. Ames, Ph.D. thesis, MIT, 2007

PMMA in compression, 140 °C



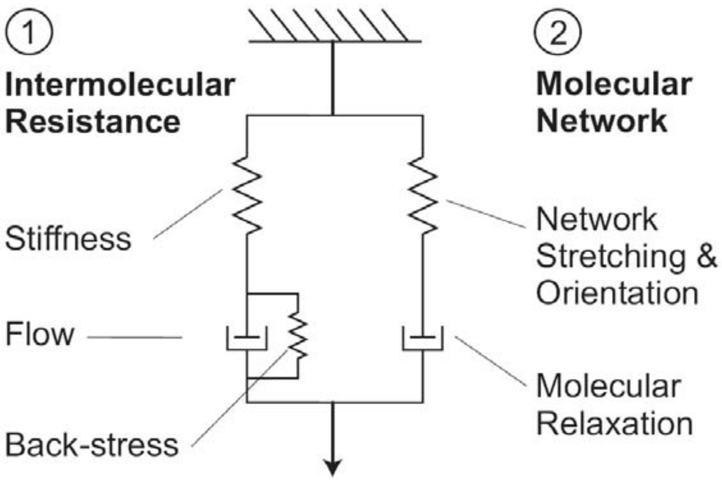
using model of N.M. Ames, Ph.D. thesis, MIT, 2007

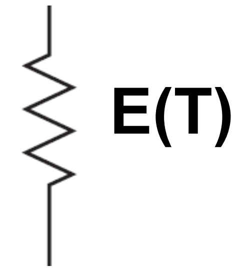
PMMA in compression (T_g = 105 °C)



using model of N.M. Ames, Ph.D. thesis, MIT, 2007

Starting point: linear elastic material model



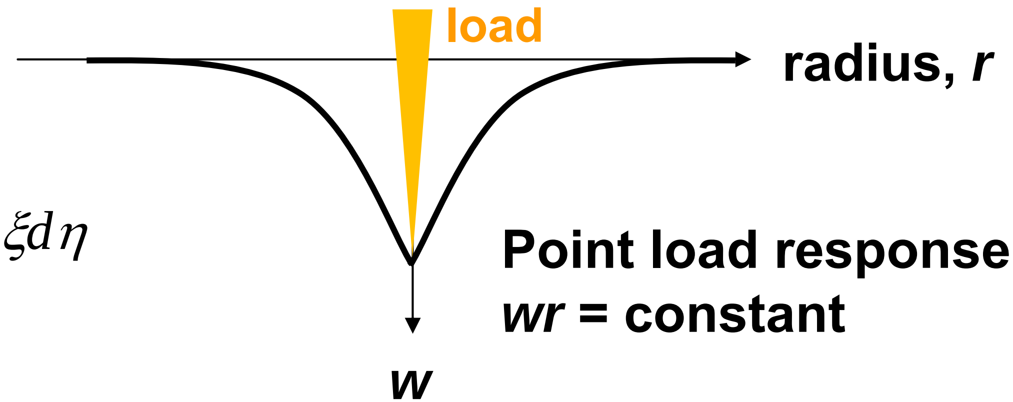


- Embossing done at high temperature, with low elastic modulus
- Deformation ‘frozen’ in place by cooling before unloading
- Wish to compute deformation of a layer when embossed with an arbitrarily patterned stamp
- Take discretized representations of stamp and substrate

Response of material to unit pressure at one location

General load response:

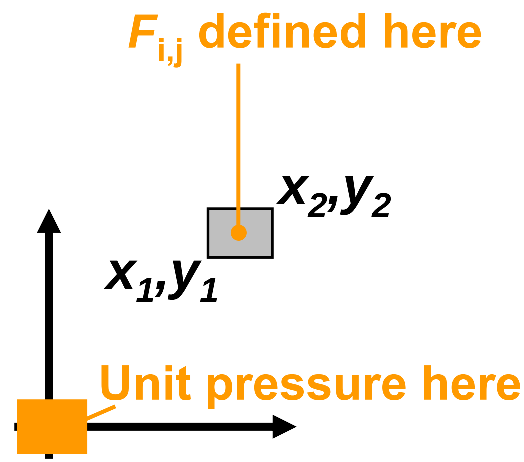
$$w(x,y) = \frac{1-\nu^2}{\pi E} \iint \frac{p(\xi,\eta)}{\sqrt{(x-\xi)^2 + (y-\eta)^2}} d\xi d\eta$$



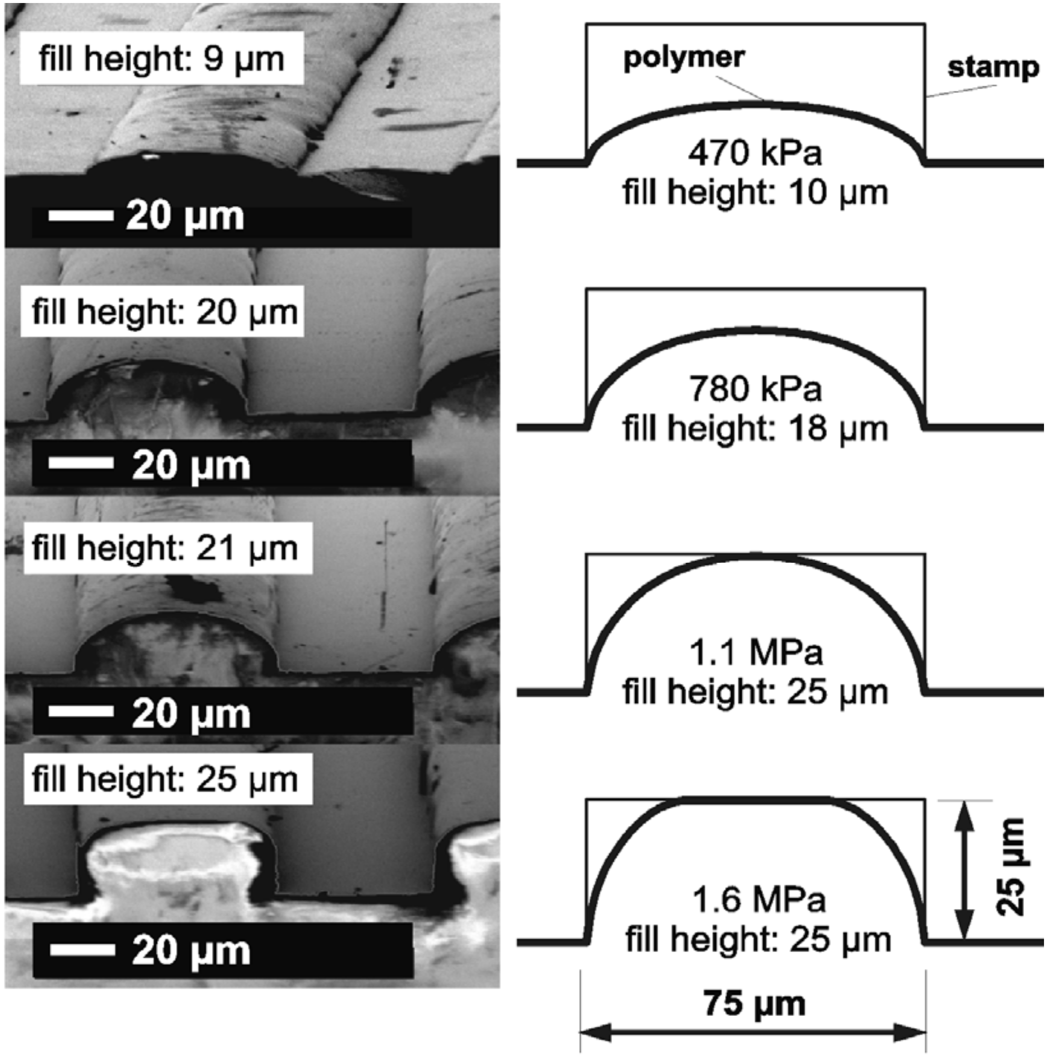
Response to unit pressure in a single element of the mesh:

$$F_{i,j} = \frac{1-\nu^2}{\pi E}\left[f(x_2,y_2) - f(x_1,y_2) - f(x_2,y_1) + f(x_1,y_1)\right]$$

$$f(x,y) = y\ln\left(x + \sqrt{x^2+y^2}\right) + x\ln\left(y + \sqrt{x^2+y^2}\right)$$



1-D verification of approach for PMMA at 130 °C

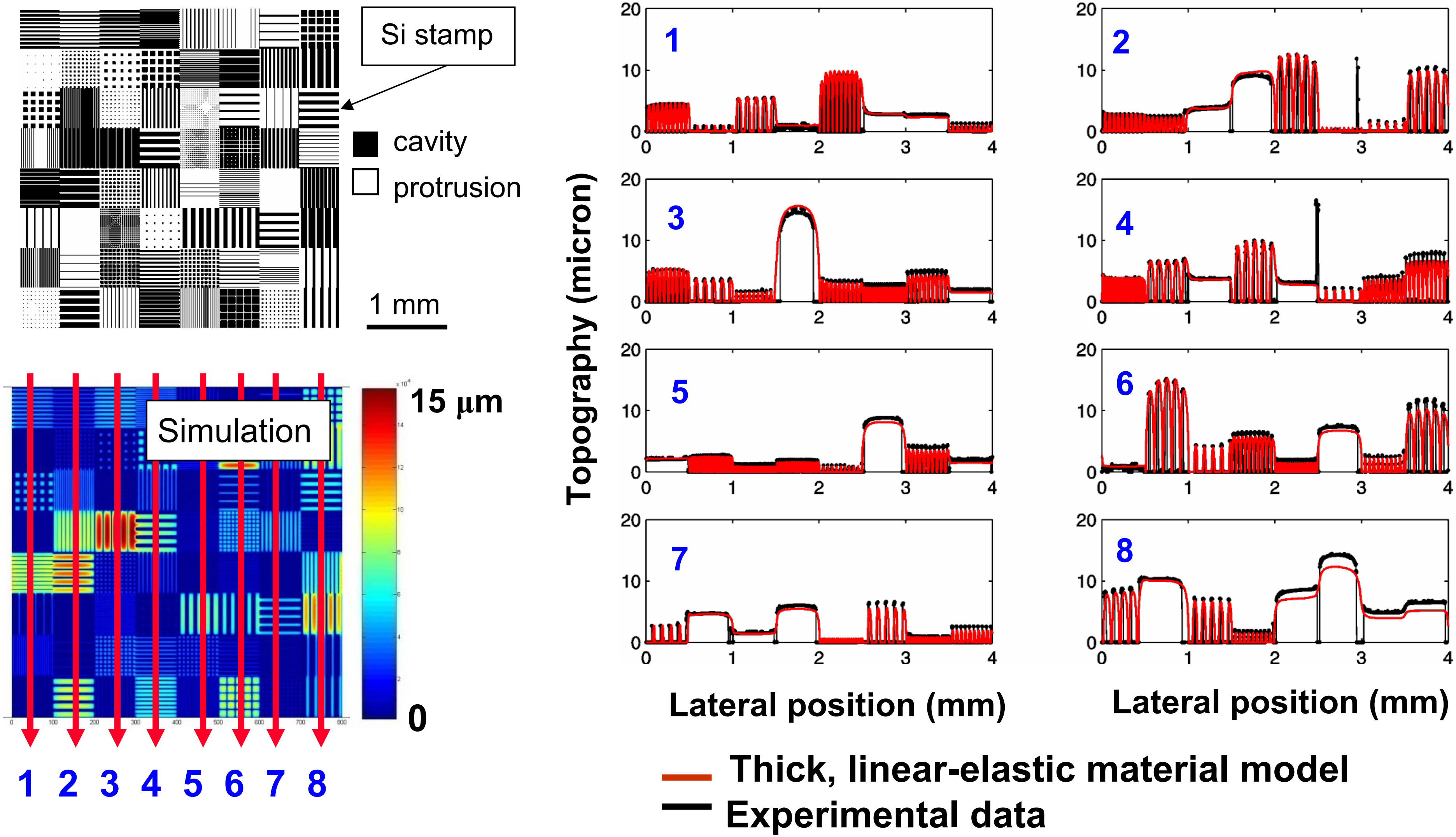


(a) experimental (b) rubbery model

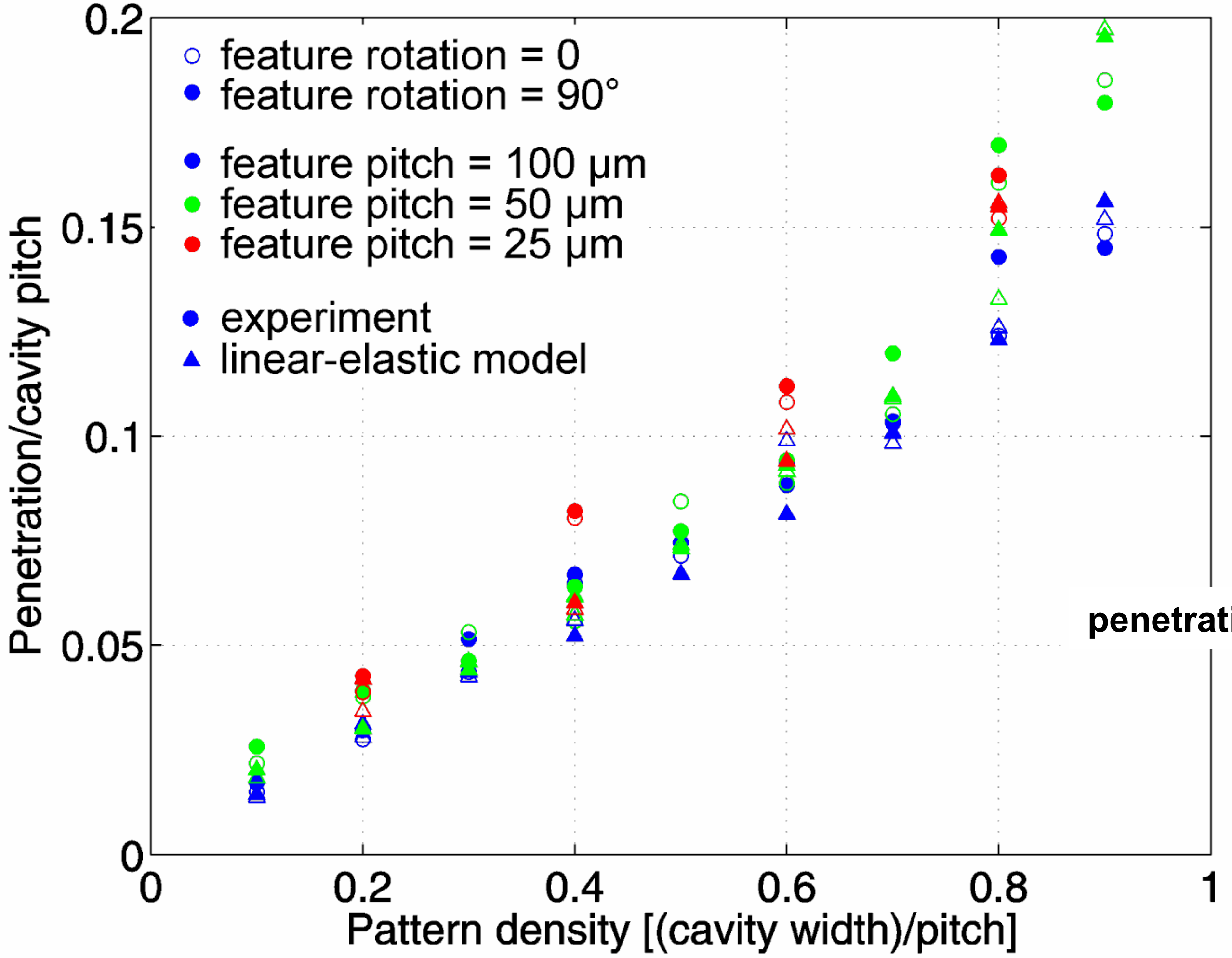
- Iteratively find distribution of pressure consistent with stamp remaining rigid while polymer deforms
- Fit elastic modulus that is consistent with observed deformations

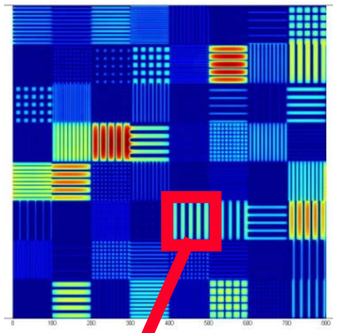
Extracted Young's modulus ~ 5 MPa at 130 °C

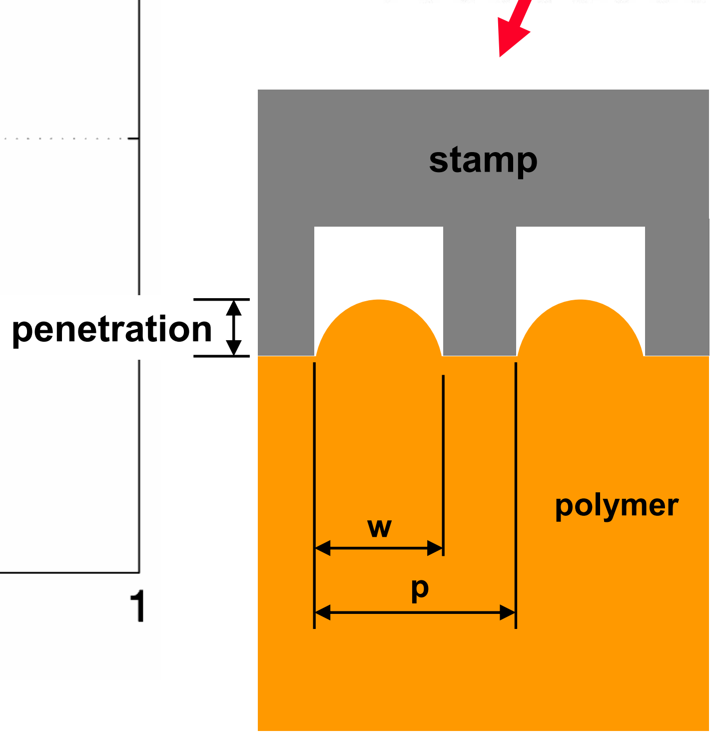
2-D linear elastic model succeeds with PMMA at 125 °C



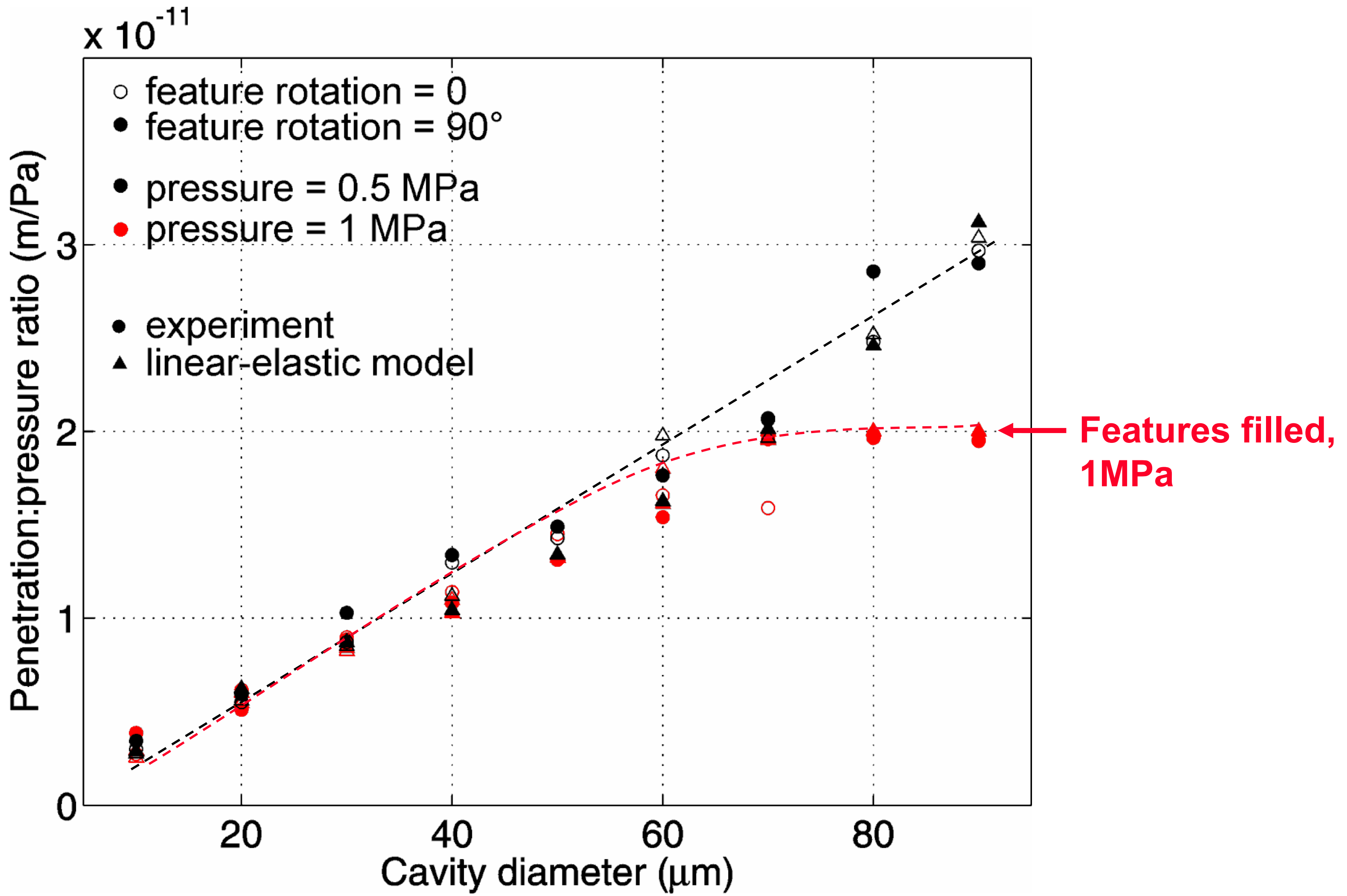
Linear-elastic model succeeds at 125 °C, p_{ave} = 0.5 MPa



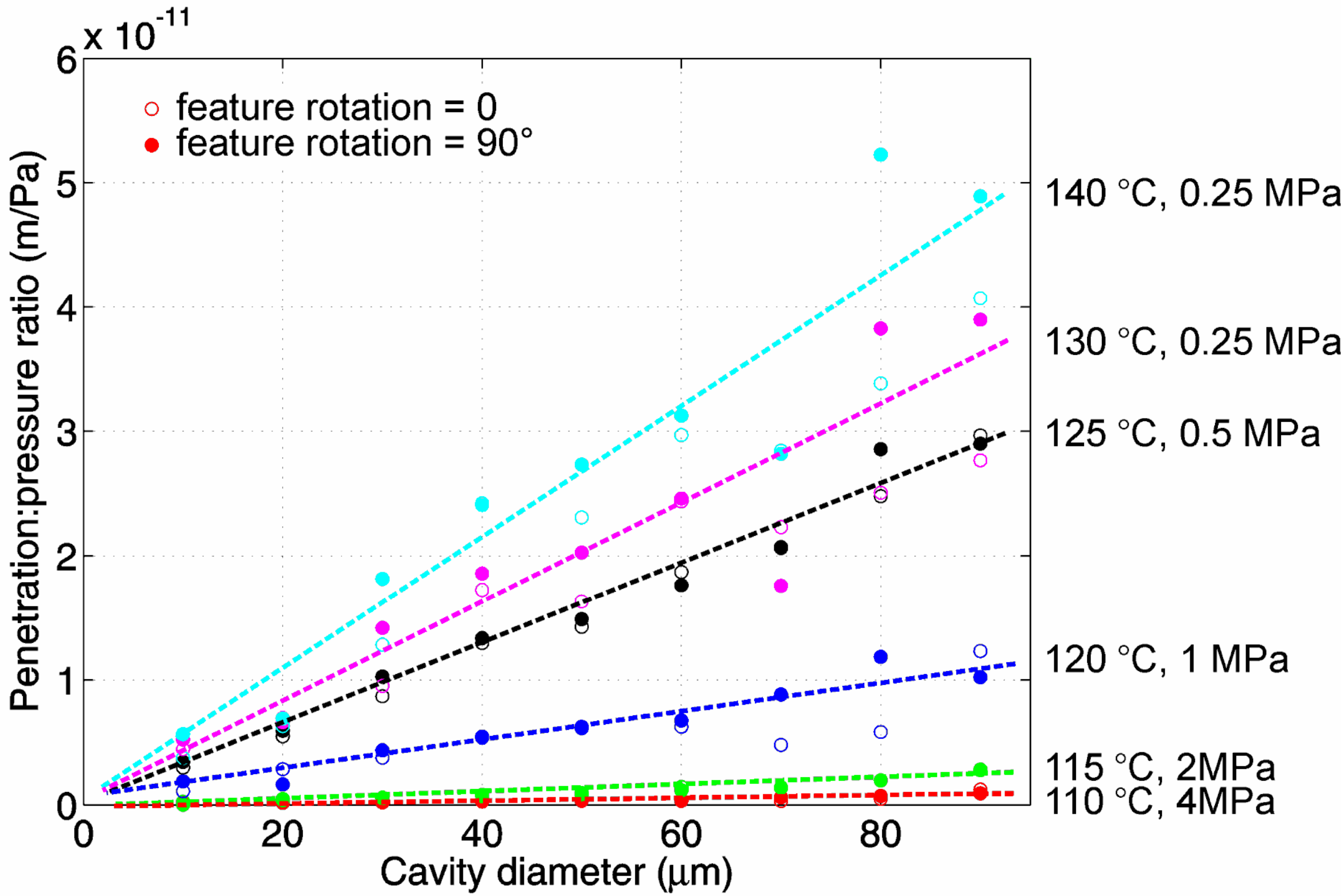




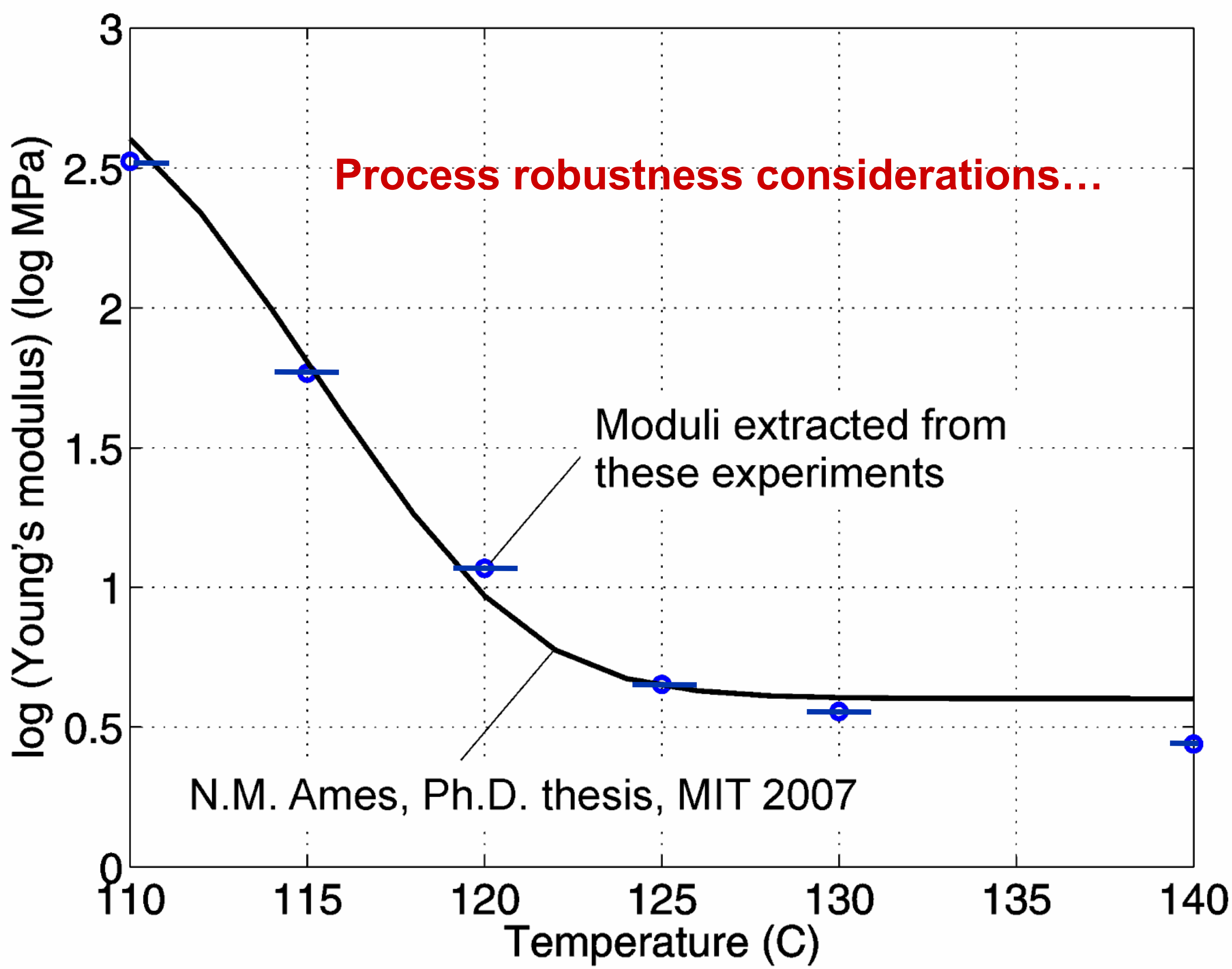
Linear-elastic model succeeds at 125 °C, p_{ave} = 1 MPa



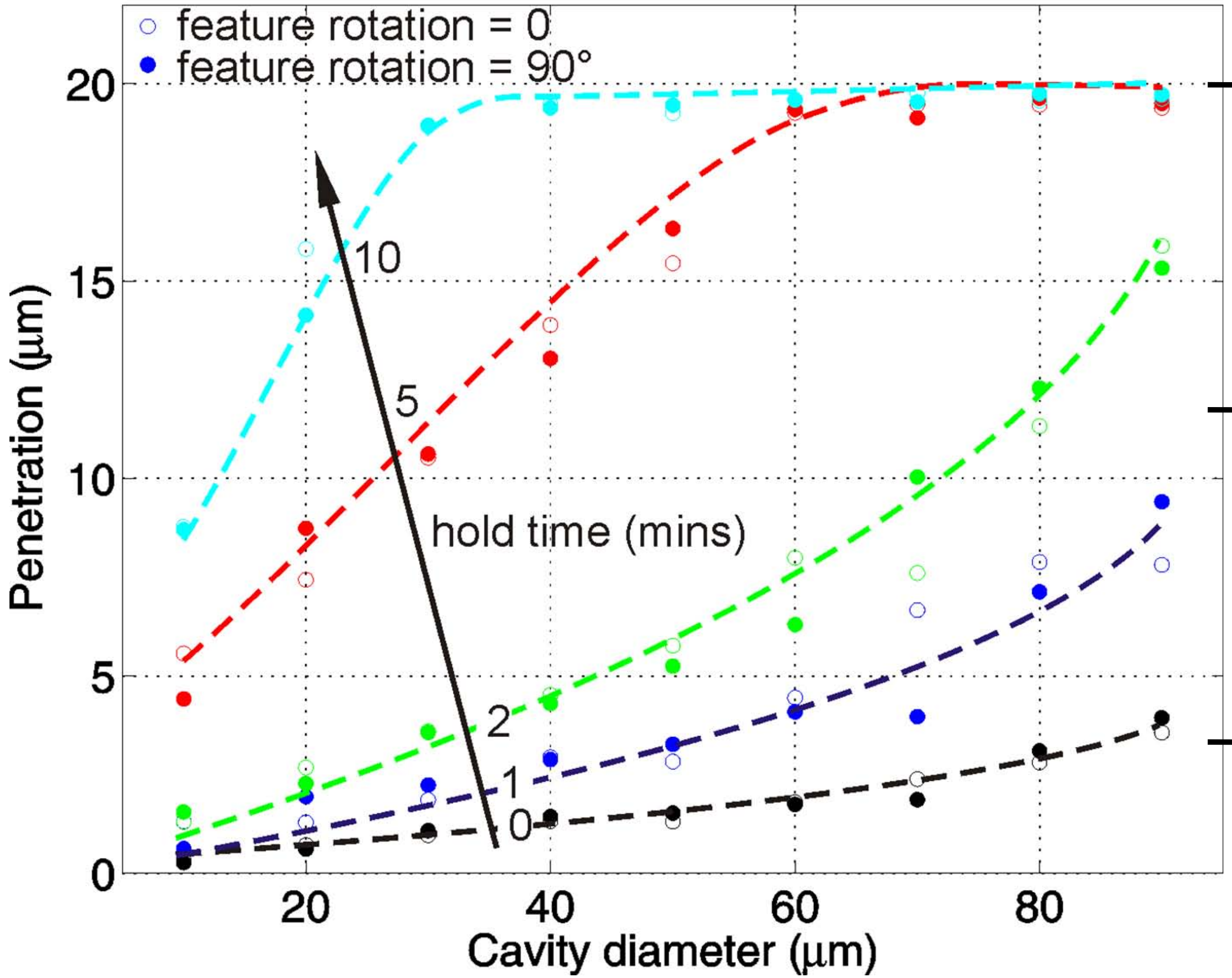
Linear elastic model succeeds below yielding at other temperatures

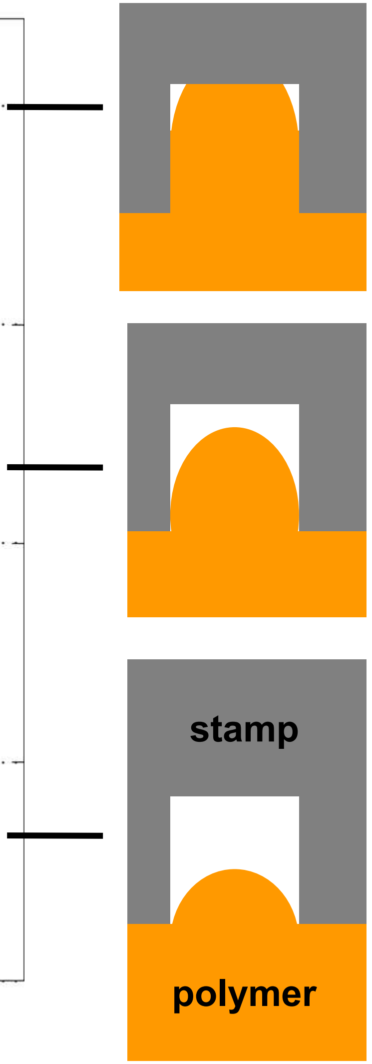


Extracted PMMA Young's moduli from 110 to 140 °C



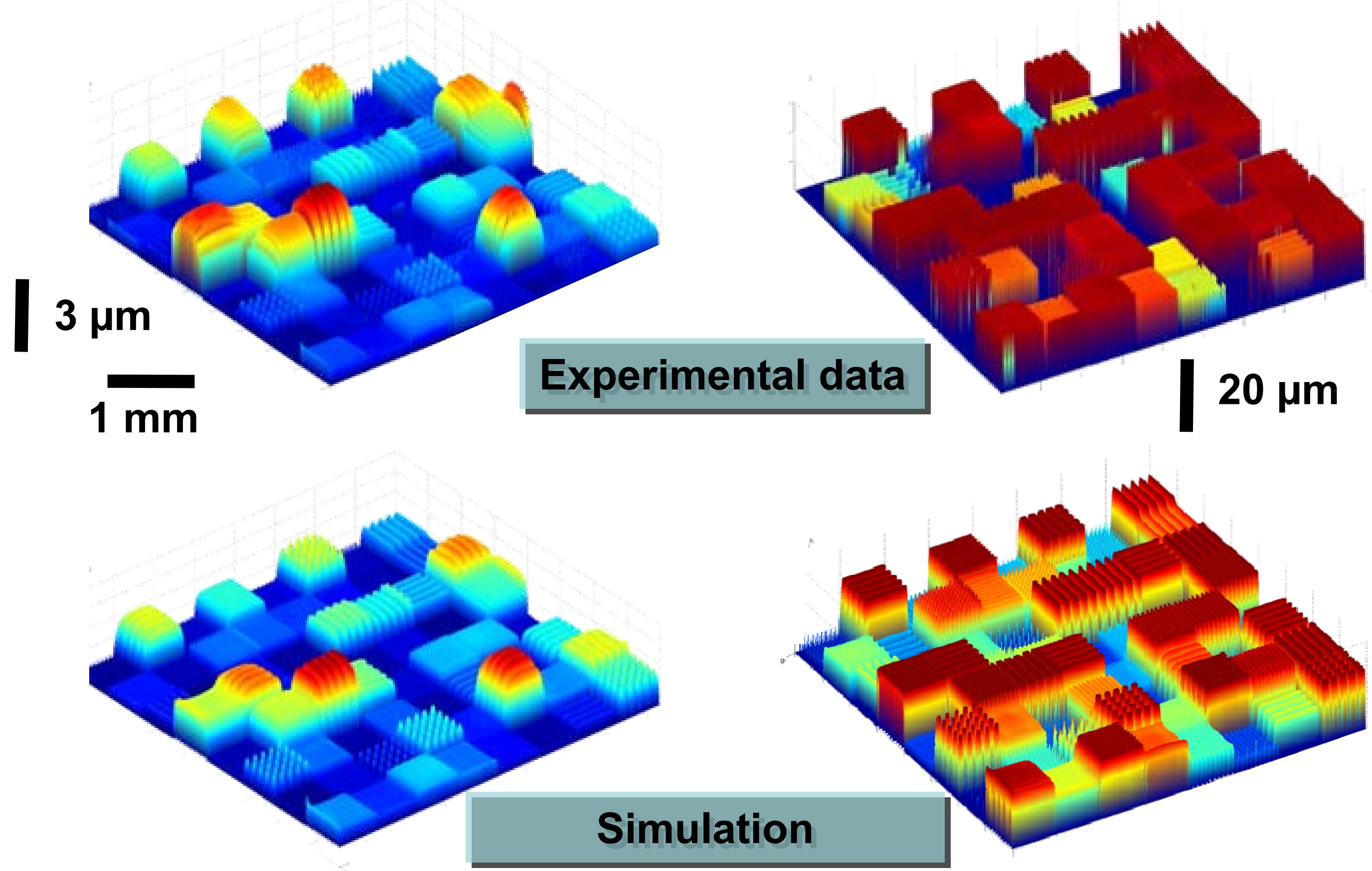
Material flows under an average pressure of 8 MPa at 110 °C





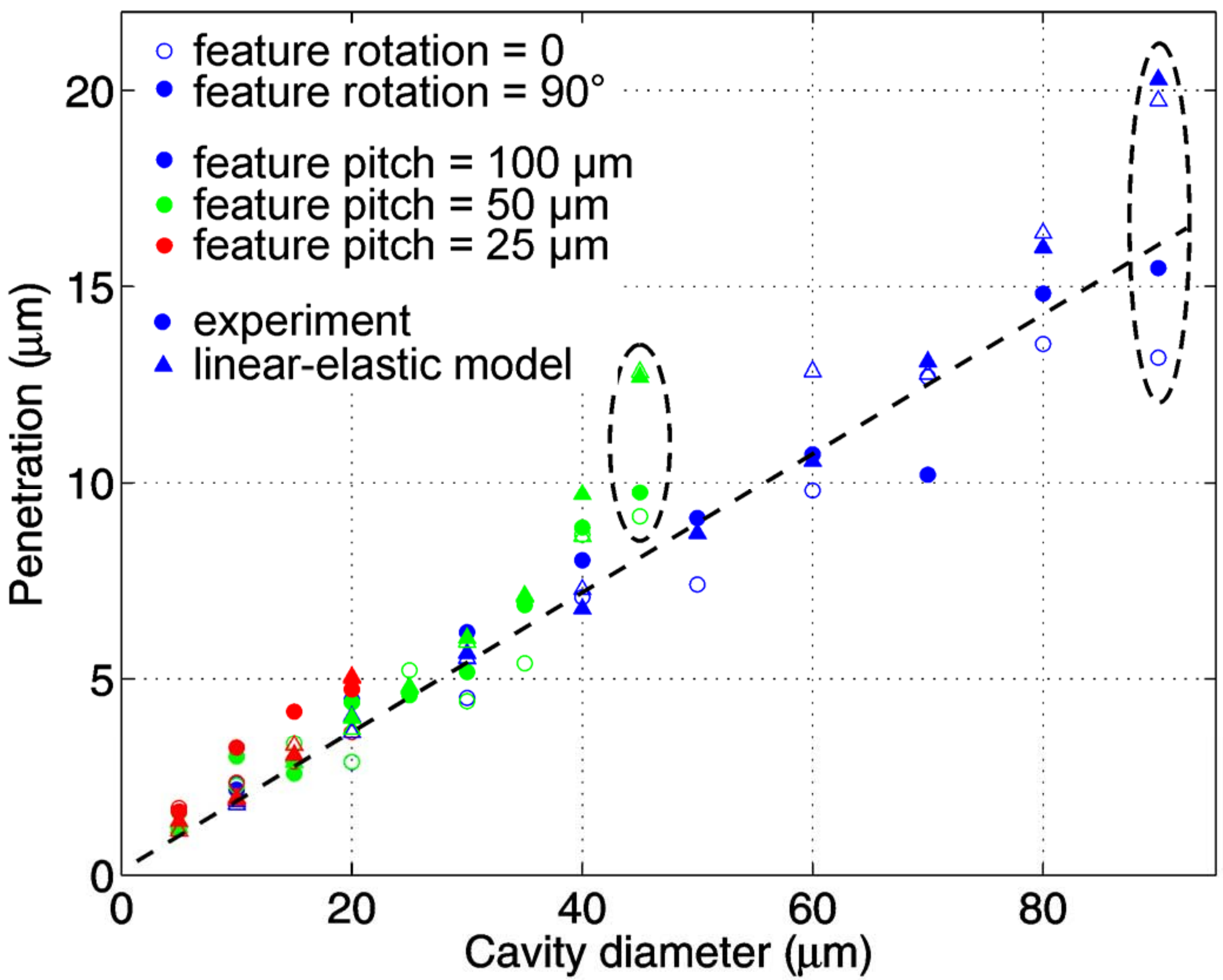
Material flows under an average pressure of 8 MPa at 110 °C

Embossed topographies (PMMA, 110 °C, 8 MPa)



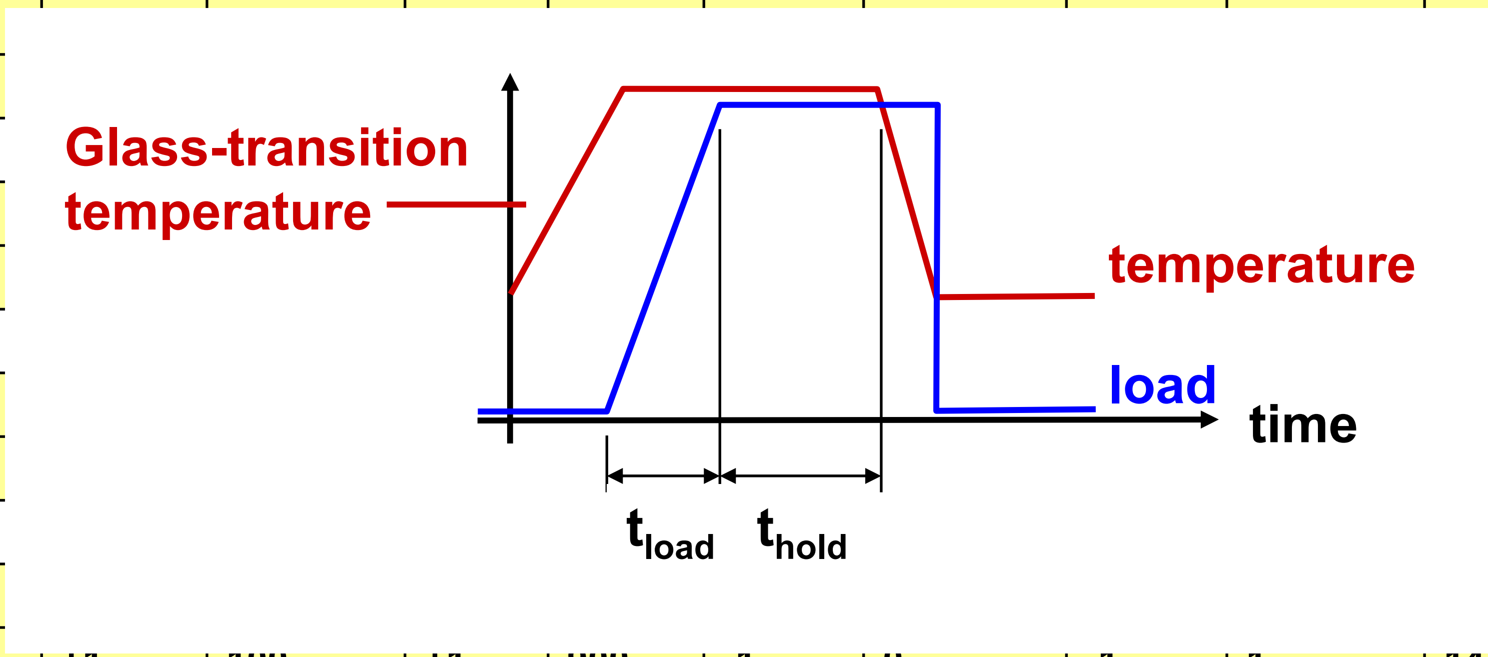
< 1 min loading time **10 mins loading time**

Zeonor 1420R embossed at 145 C

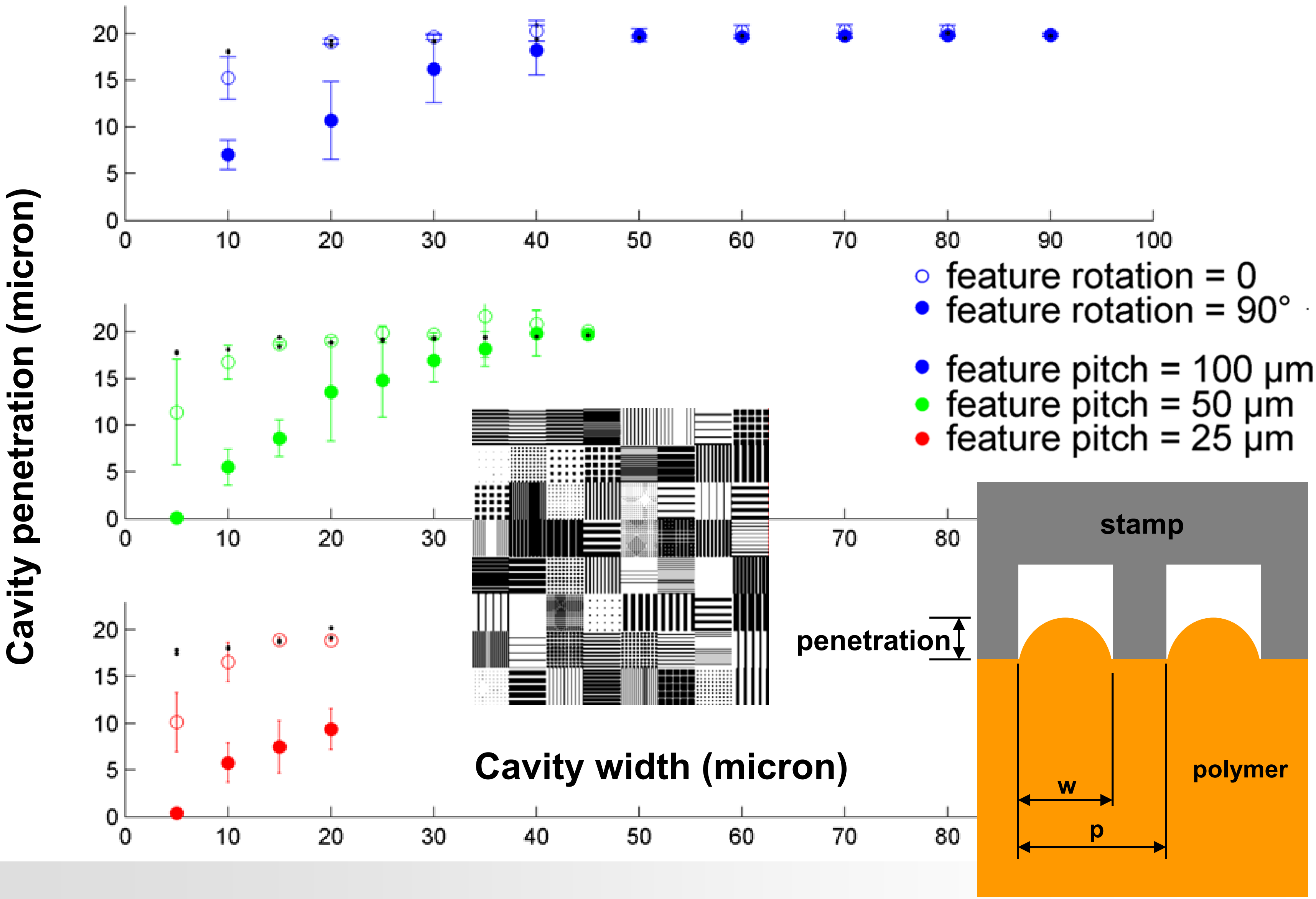


2^{4-1}_{IV} experimental design with replicated centerpoints

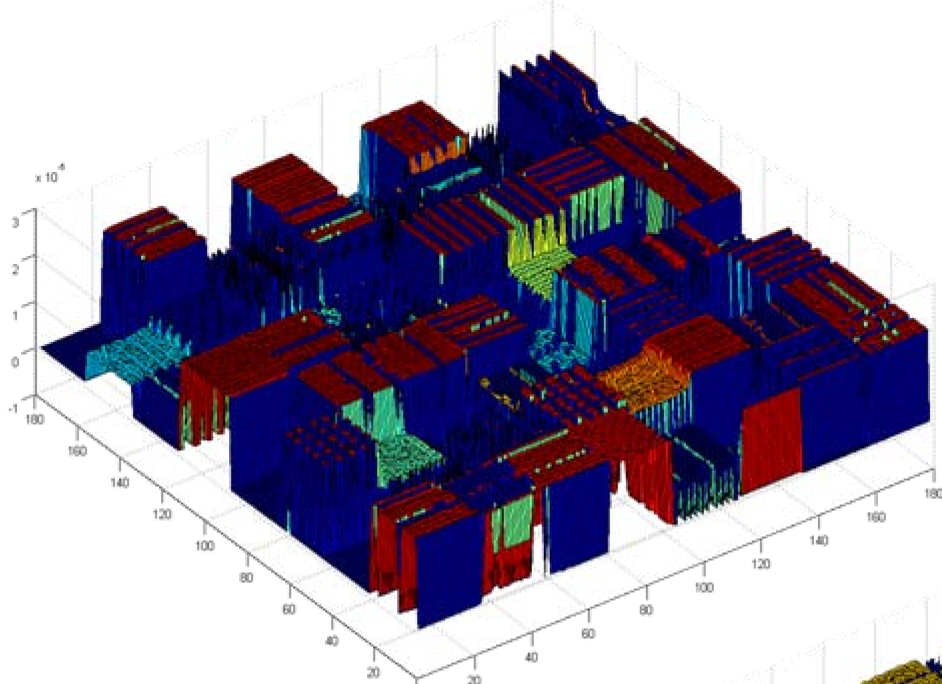
Sample	Temp	Temp/C	Force	Force /N	Hold	Hold /min	Rate	Time to load (s)	Mean penetration (microns)
P352	0	95	0	500	0	4	0	10	14.100
P353									.408
P354									.721
P355									.216
P356									.973
P357									.217
P358									.725
P359									157
P360									563
P361									.454
P362									.912
P363	+1	100	+1	900	-1	0	-1	1	14.014
P364	0	95	0	500	0	4	0	10	14.291



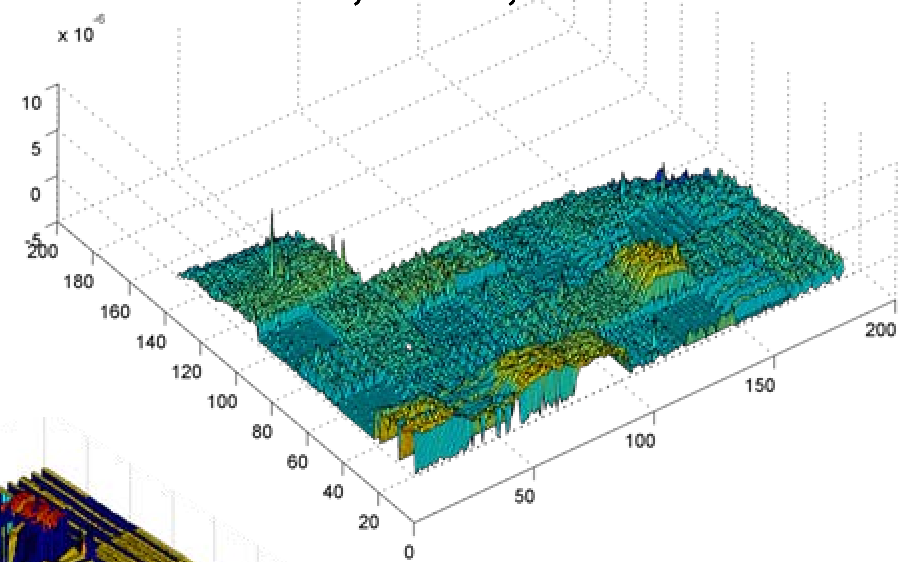
Topas 5013 ‘centerpoint’ runs



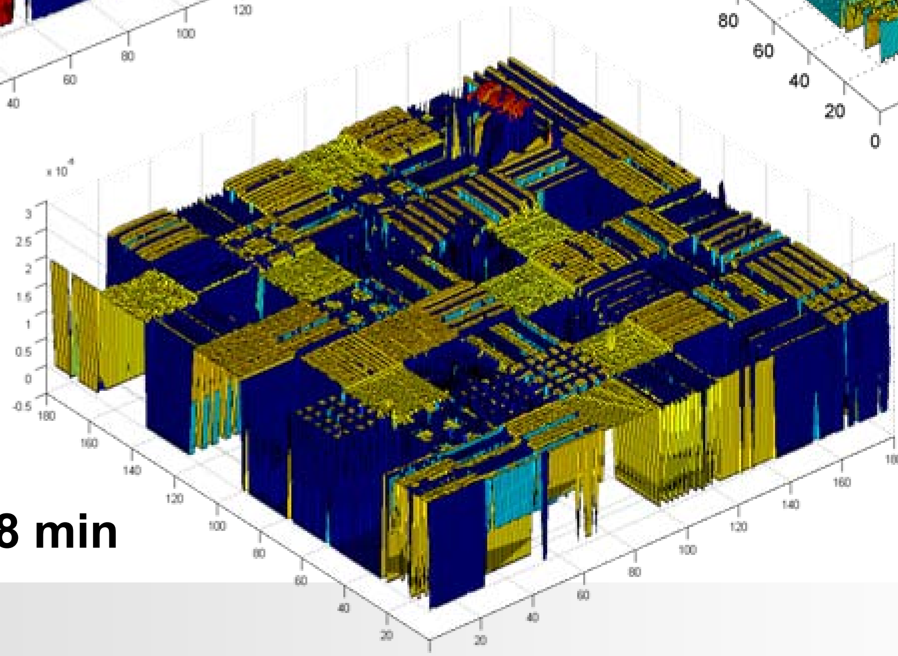
Topas 5013 embossed under three sets of conditions



95 C, 500 N, 4 min



90 C, 100 N, 8 min



100 C, 900 N, 8 min

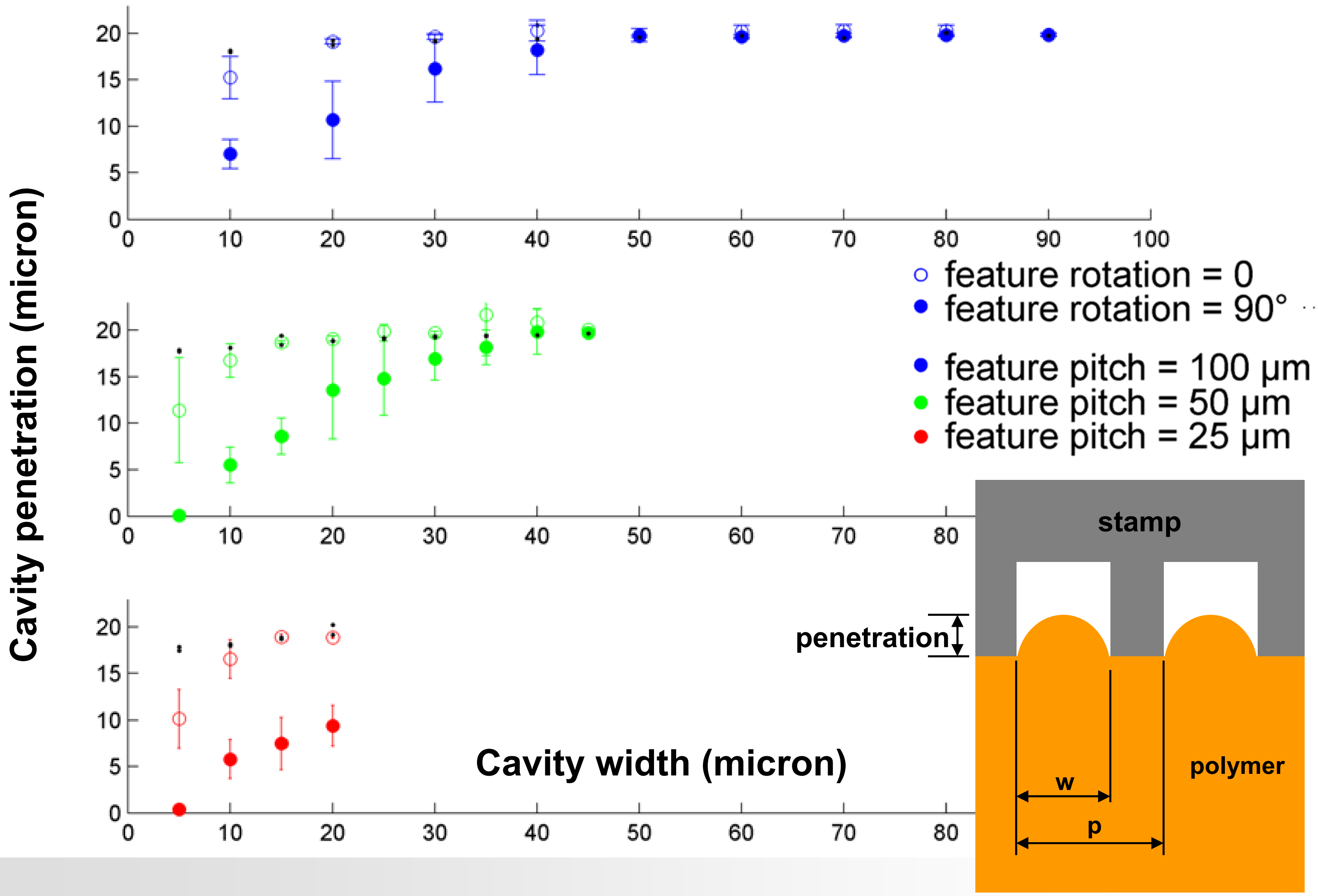
2^{4-1}_{IV} experimental design with replicated centerpoints

Sample	Temp	Temp/C	Force	Force /N	Hold	Hold /min	Rate	Time to load (s)	Mean penetration (microns)
P352	0	95	0	500	0	4	0	10	14.100
P353	-1	90	+1	900	+1	8	-1	1	16.408
P354	-1	90	-1	100	-1	0	-1	1	4.1721
P355	0	95	0	500	0	4	0	10	16.216
P356	+1	100	-1	100	+1	8	-1	1	12.973
P357	-1	90	+1	900	-1	0	+1	19	13.217
P358	0	95	0	500	0	4	0	10	13.725
P359	+1	100	-1	100	-1	0	+1	19	7.3157
P360	-1	90	-1	100	+1	8	+1	19	2.4563
P361	0	95	0	500	0	4	0	10	14.454
P362	+1	100	+1	900	+1	8	+1	19	18.912
P363	+1	100	+1	900	-1	0	-1	1	14.014
P364	0	95	0	500	0	4	0	10	14.291

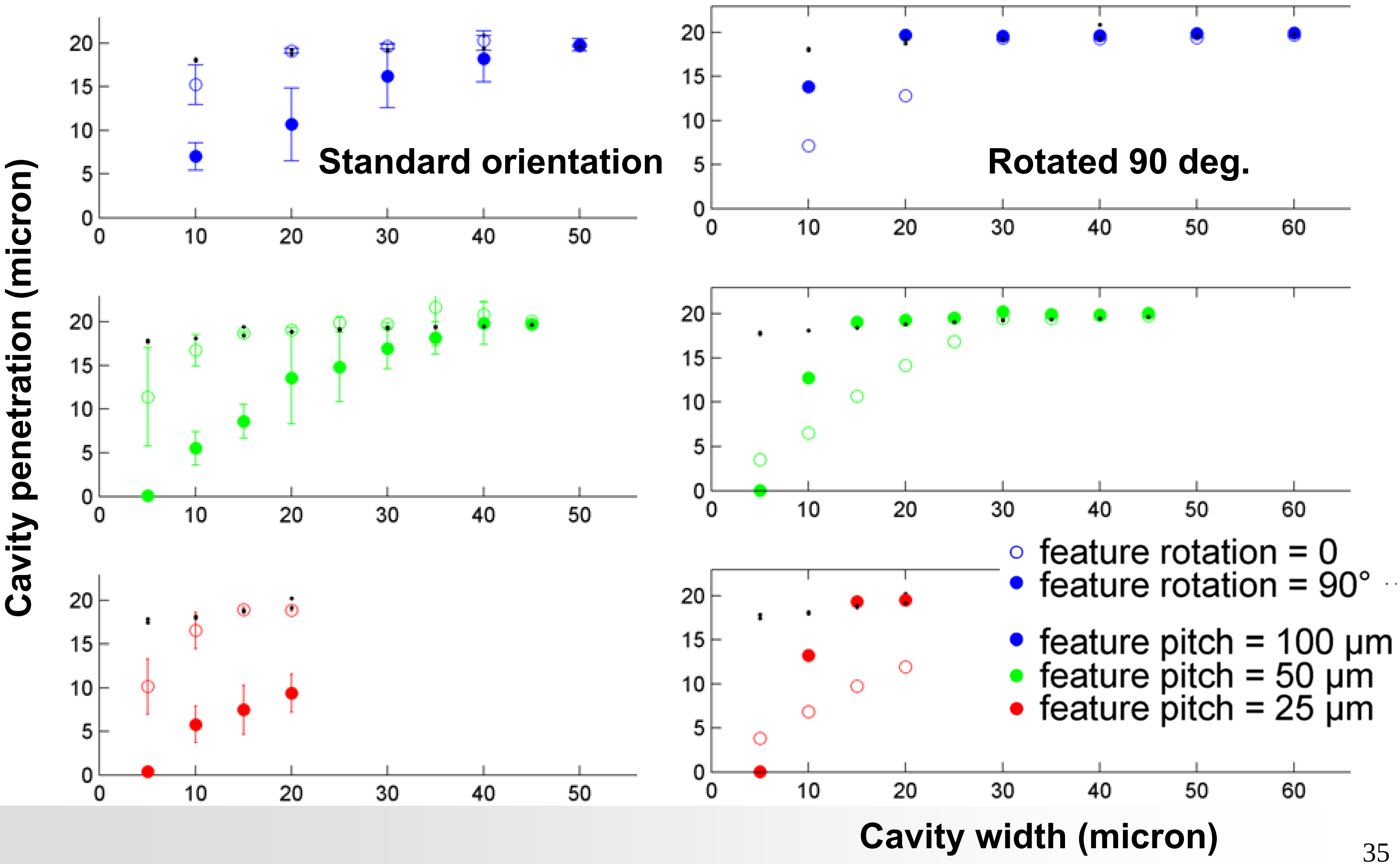
ANOVA for Topas 5013 embossing experiments

	Source of variation	SS	dof	MS	F0	P-value	
Temp	A	35.9607	1	35.9607	48.0822	0.00096	alias BCD
Force	B	158.722	1	158.722	212.223	2.8E-05	alias ACD
	AB	13.4144	1	13.4144	17.936	0.00821	alias CD
Hold time	C	18.0916	1	18.0916	24.1898	0.0044	alias ABD
	AC	10.306	1	10.306	13.7799	0.01382	alias BD
	BC	2.15022	1	2.15022	2.875	0.15073	alias AD
Load rate	D	4.01309	1	4.01309	5.3658	0.06836	alias ABC
	Quadratic	39.316	1	39.316	52.5684	0.00078	
	Error	3.73951	5	0.7479			
	Total		13				

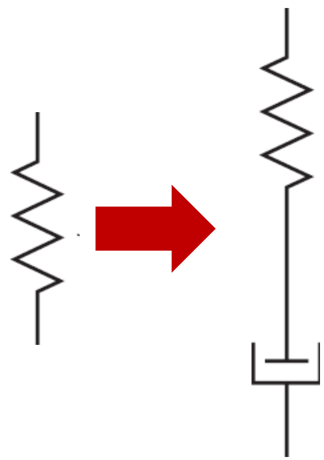
Topas 5013 ‘centerpoint’ runs

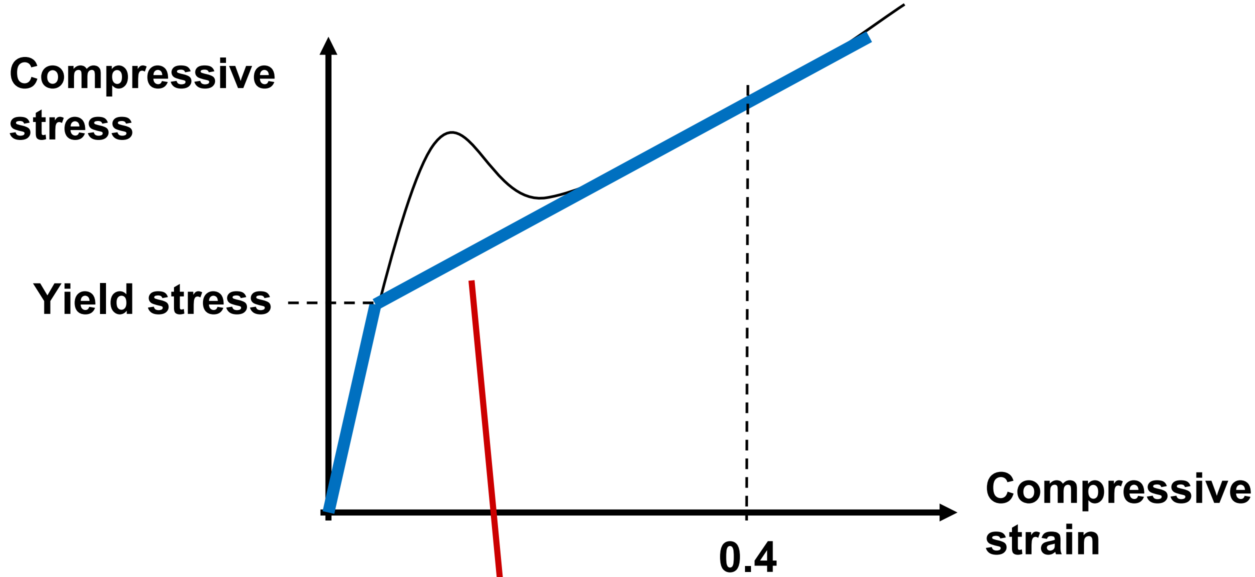


Topas 5013 centerpoint run, rotated 90 degrees: shows substrate anisotropy



Modelling combined elastic/plastic behavior





Plastic flow

Deborah number
De = $t_{material}/t_{load,\ hold}$

De << 1

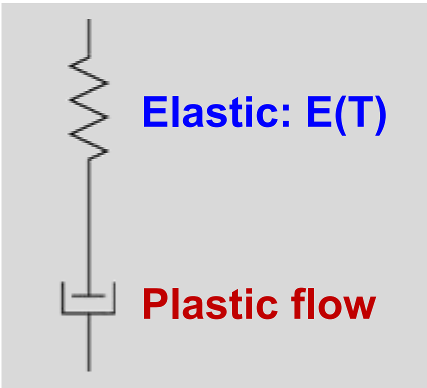
De ~ 1

De >> 1

Consider plastic deformation instantaneous

Consider flow to be measurable but not to modify the pressure distribution substantially during hold

Modelling combined elastic/plastic behavior



Plastic flow

De << 1

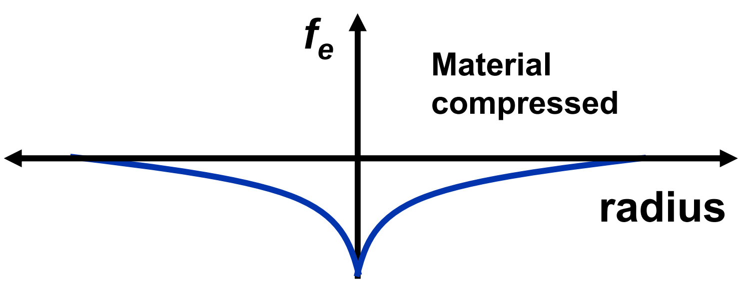
De ~ 1

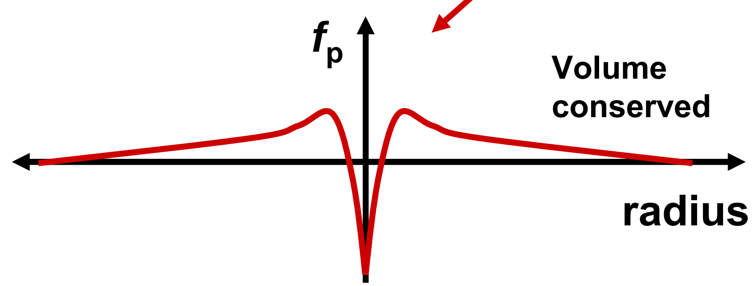
De >> 1

$$w(x,y) = p(x,y) * f_e(x,y) + \left[p(x,y) - p_{yield} \right] * \left(A + \overline{Bt_{hold}} \right) f_p(x,y)$$

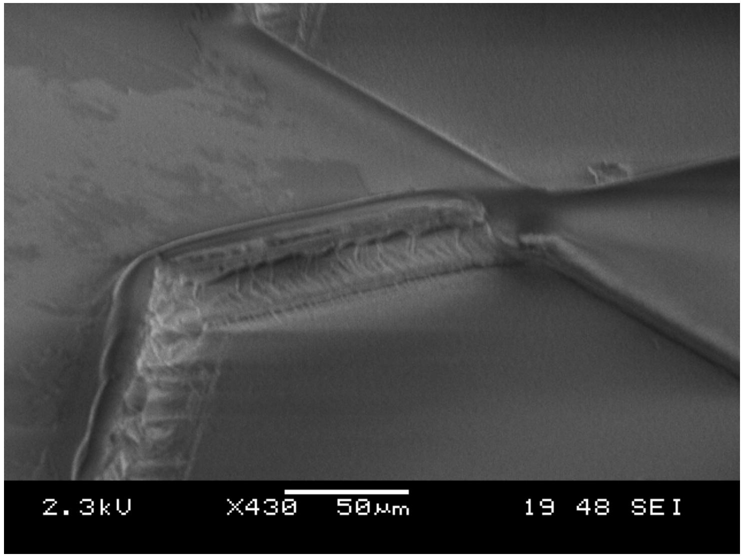
Existing linear-elastic component

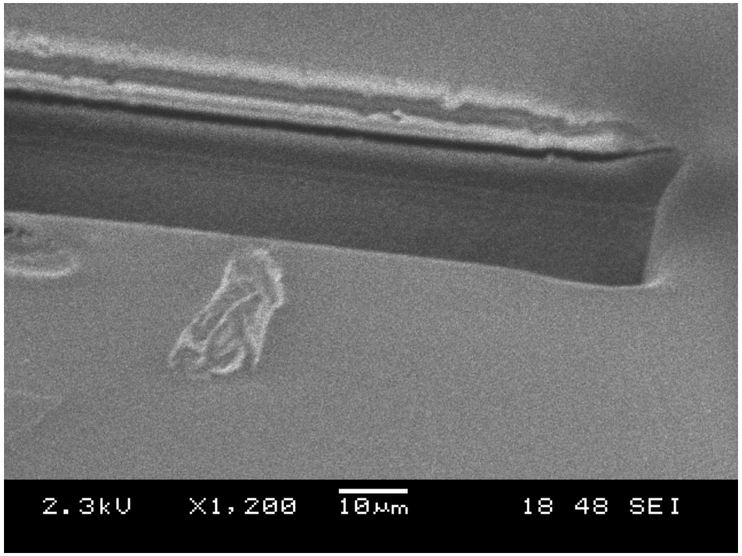
Tuned to represent cases from capillary filling to non-slip Poiseuille flow



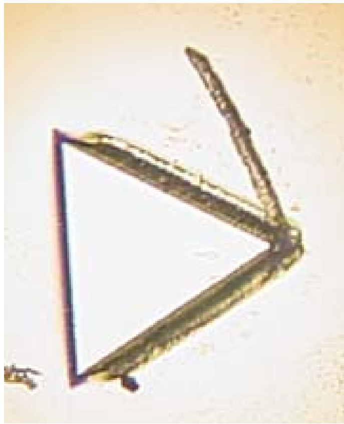


Differential thermal expansion gives rise to workpiece- *and* feature-scale non-uniformity

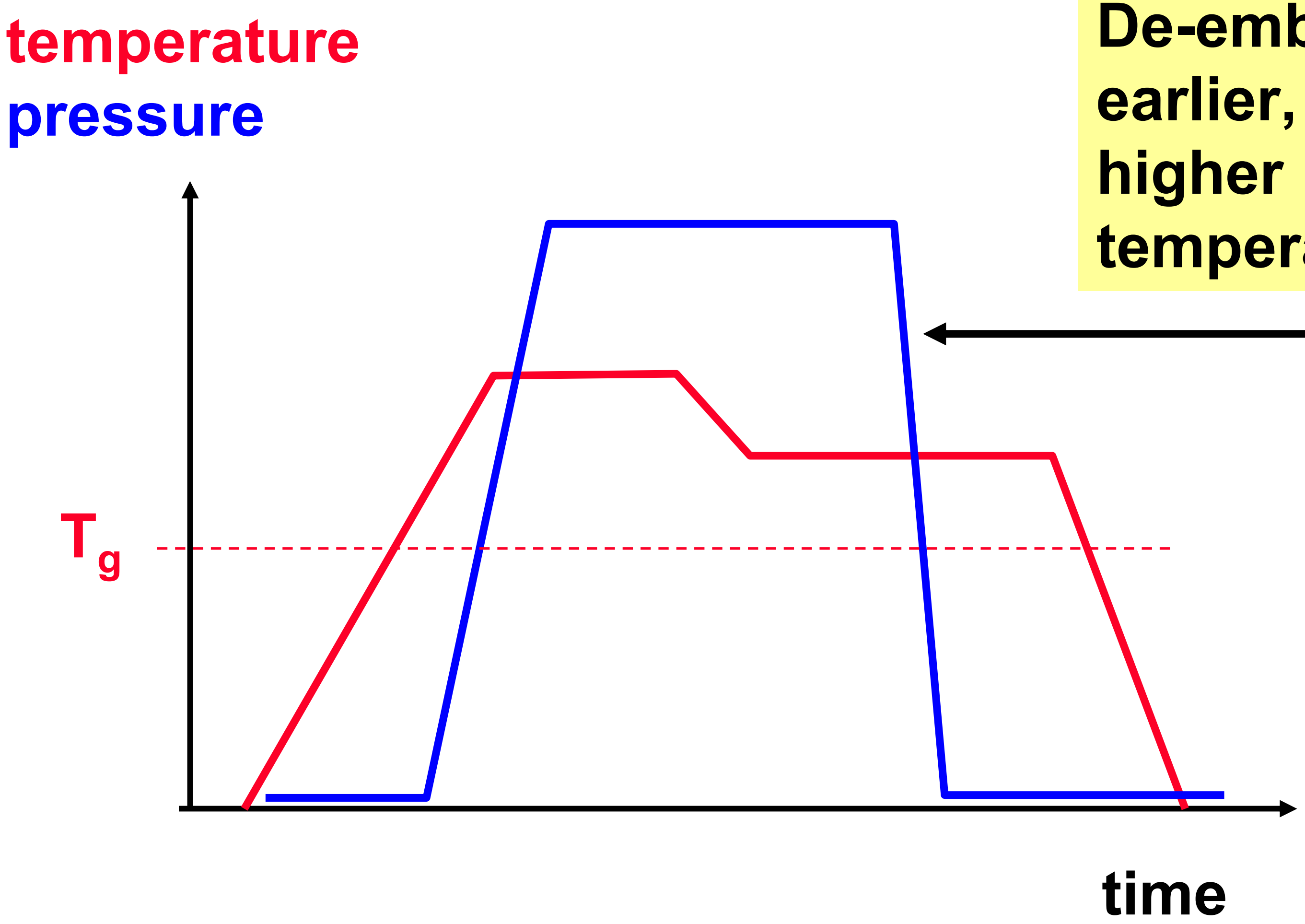




'Ploughing' in plastic caused by differential thermal contraction of Si mold and polymer substrate (embossing at ~130 °C)

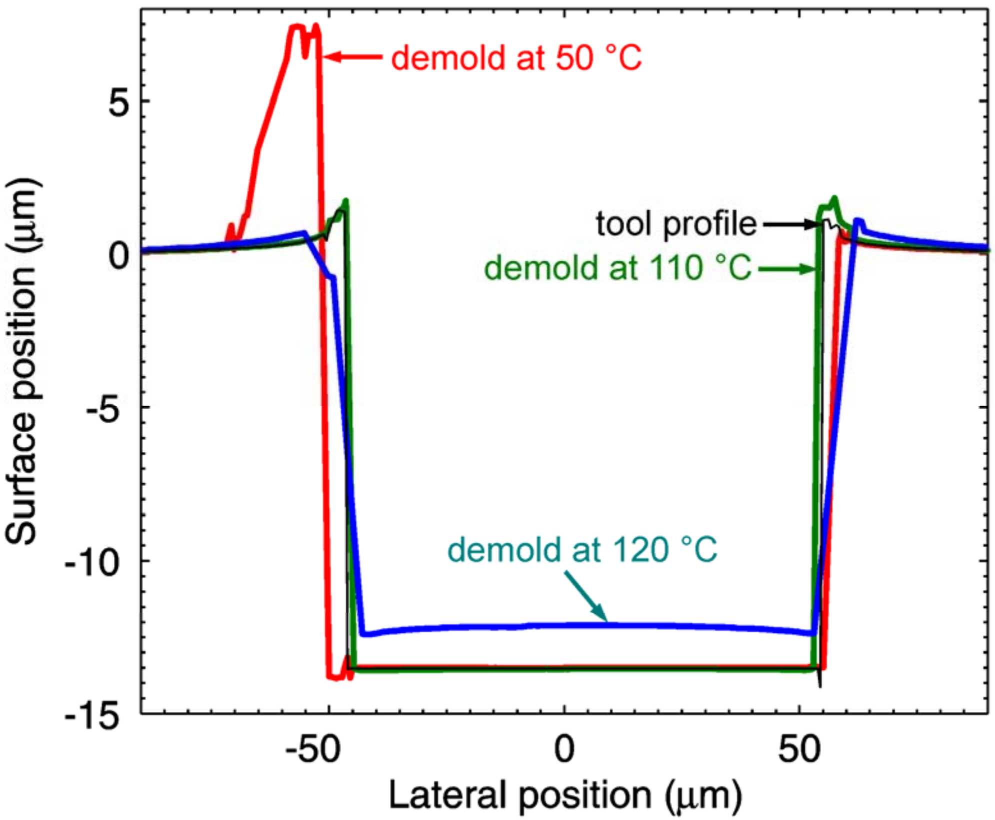


Modifying the process: hot demolding



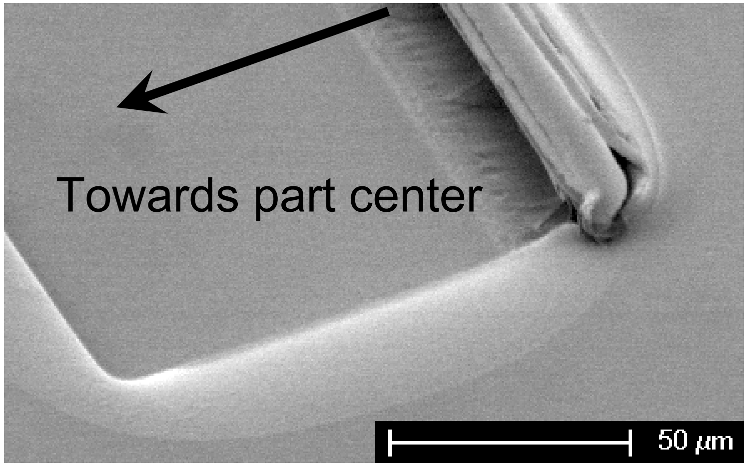
De-emboss earlier, at higher temperature?

‘Ploughing’ avoided by hot demolding

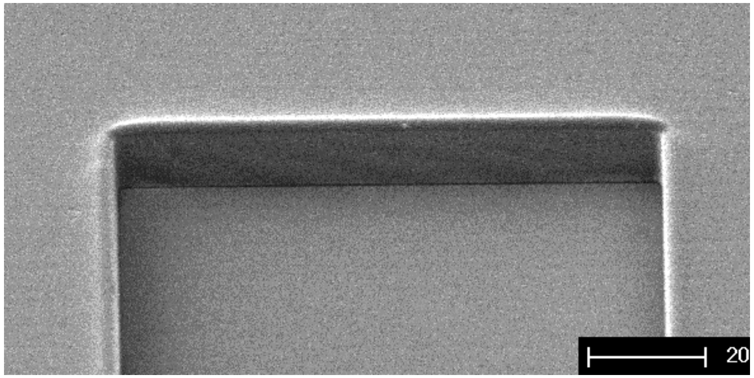


Cross-sections of 100 μm wide by 15 μm-deep square.
Obtained by scanning white-light interferometry.

Process robustness considerations…
traded off with performance

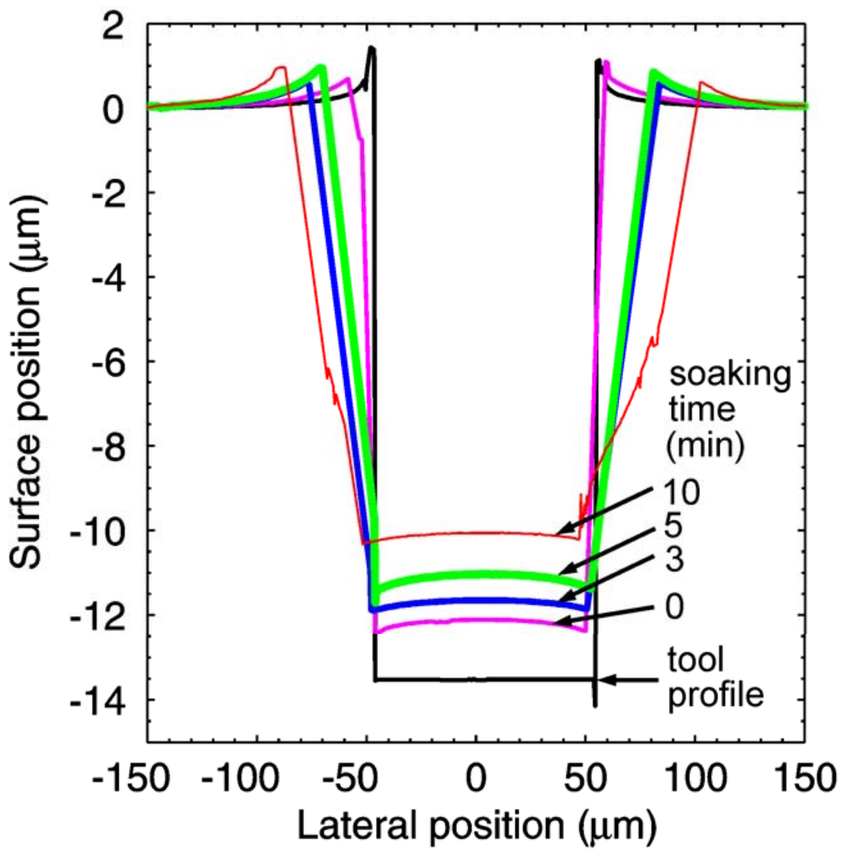


SEM of end of 100 μm wide by 15 μm-deep trench, de-molded at 50 °C

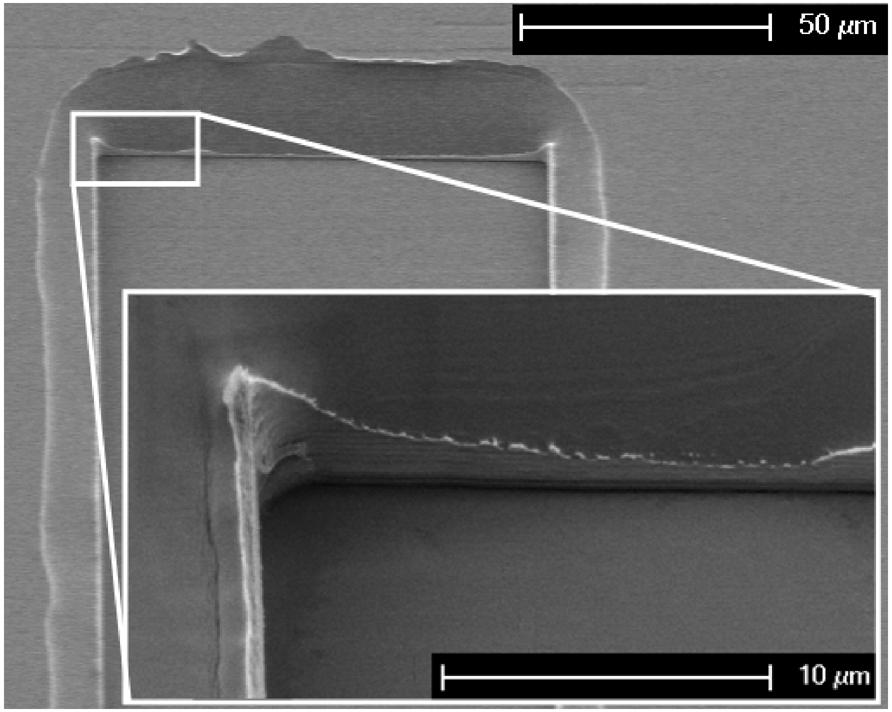


SEM of end of 100 μm wide by 15 μm-deep trench, de-molded at 110 ° C

Typical embossed features spring and creep back over several minutes



Cross-sections of 100 µm wide by 15 µm-deep square. Obtained by scanning white-light interferometry.



SEM of end of 100 µm wide x 15 µm deep channel, de-molded at 120 °C after 10 minutes